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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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NEWS 3	APR 02	PATDPAFULL: Application and priority number formats enhanced
NEWS 4	APR 02	DWPI: New display format ALLSTR available
NEWS 5	APR 02	New Thesaurus Added to Derwent Databases for Smooth Sailing through U.S. Patent Codes
NEWS 6	APR 02	EMBASE Adds Unique Records from MEDLINE, Expanding Coverage back to 1948
NEWS 7	APR 07	CA/CAplus CLASS Display Streamlined with Removal of Pre-IPC 8 Data Fields
NEWS 8	APR 07	50,000 World Traditional Medicine (WTM) Patents Now Available in CAplus
NEWS 9	APR 07	MEDLINE Coverage Is Extended Back to 1947
NEWS 10	JUN 16	WPI First View (File WPIFV) will no longer be available after July 30, 2010
NEWS 11	JUN 18	DWPI: New coverage - French Granted Patents
NEWS 12	JUN 18	CAS and FIZ Karlsruhe announce plans for a new STN platform
NEWS 13	JUN 18	IPC codes have been added to the INSPEC backfile (1969-2009)
NEWS 14	JUN 21	Removal of Pre-IPC 8 data fields streamline displays in CA/CAplus, CASREACT,and MARPAT
NEWS 15	JUN 21	Access an additional 1.8 million records exclusively enhanced with 1.9 million CAS Registry Numbers -- EMBASE Classic on STN
NEWS 16	JUN 28	Introducing "CAS Chemistry Research Report": 40 Years of Biofuel Research Reveal China Now Atop U.S. in Patenting and Commercialization of Bioethanol
NEWS 17	JUN 29	Enhanced Batch Search Options in DGENE, USGENE, and PCTGEN
NEWS 18	JUL 19	Enhancement of citation information in INPADOC databases provides new, more efficient competitor analyses
NEWS 19	JUL 26	CAS coverage of global patent authorities has expanded to 61 with the addition of Costa Rica

NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
AND CURRENT DISCOVER FILE IS DATED 07 JULY 2010.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:43:17 ON 19 AUG 2010

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.08	3.08

FILE 'REGISTRY' ENTERED AT 14:51:24 ON 19 AUG 2010

Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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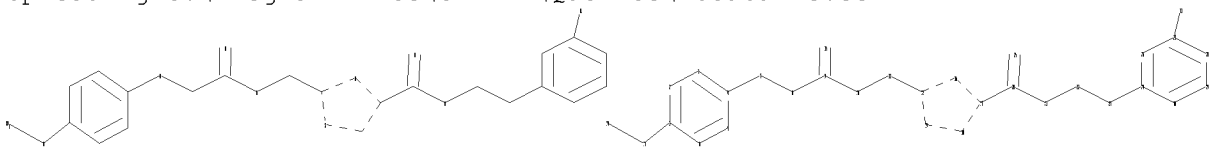

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7  8  9  10  11  13  14  15  20  21  22  23  25  31
ring nodes :
1  2  3  4  5  6  12  16  17  18  19  24  26  27  28  29  30
chain bonds :
1-13  4-7  7-8  8-9  9-10  9-15  10-11  11-12  13-14  17-20  20-21  20-25  21-22
22-23  23-24  27-31
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  12-16  12-19  16-17  17-18  18-19  24-26  24-30
26-27  27-28  28-29  29-30
exact/norm bonds :
1-13  4-7  7-8  9-10  9-15  10-11  12-16  12-19  16-17  17-18  18-19  20-21  20-25
21-22
exact bonds :
8-9  11-12  13-14  17-20  22-23  23-24  27-31
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  24-26  24-30  26-27  27-28  28-29  29-30


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
 11:CLASS  12:Atom  13:CLASS  14:CLASS  15:CLASS  16:Atom  17:Atom  18:Atom
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27:Atom  28:Atom  29:Atom  30:Atom  31:CLASS



L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 14:51:44 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       21 TO ITERATE

100.0% PROCESSED       21 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          146 TO      694
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 14:51:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      411 TO ITERATE

100.0% PROCESSED      411 ITERATIONS                                4 ANSWERS
SEARCH TIME: 00.00.01

L3            4 SEA SSS FUL L1

=> fil caplus
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	191.54	194.62

FILE 'CAPLUS' ENTERED AT 14:51:50 ON 19 AUG 2010
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FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010 (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

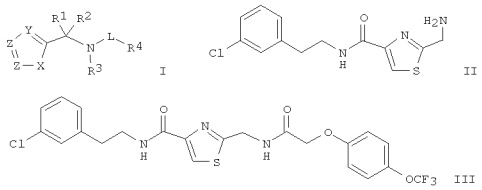
=> d ibib abs hitstr tot

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:1126676 CAPLUS
DOCUMENT NUMBER: 143:405899
TITLE: Preparation of thiazoles and analogs as anaplastic lymphoma kinase modulators
INVENTOR(S): Leahy, James William; Lewis, Gary Lee; Nuss, John M.; Ridgway, Brian Hugh; Sangalang, Joan C.
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 346 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005097765	A1	20051020	WO 2005-US10969	20050331
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005230847	A1	20051020	AU 2005-230847	20050331
CA 2559866	A1	20051020	CA 2005-2559866	20050331
EP 1730128	A1	20061213	EP 2005-733275	20050331
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2008502595	T	20080131	JP 2007-506579	20050331
US 20090186905	A1	20090723	US 2007-598911	20070607
PRIORITY APPLN. INFO.:			US 2004-558800P P	20040331
			WO 2005-US10969 W	20050331

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 143:405899; MARPAT 143:405899
GI

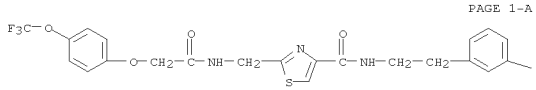


AB Title compds. I [wherein R1, R2 = H, halo, trihalomethyl; R1 and R2 are oxo; R3, R4 = H, (un)substituted alkyl, aryl; X = O, S; Y = (un)substituted CH or N; one of Z = C(COO-alkyl), C(CONH-alkyl), while the other Z = N, (un)substituted CH; L = C(O/S), SO2 or absence; etc., pharmaceutically acceptable salts, hydrates or prodrugs thereof] as modulators of protein kinases, especially anaplastic lymphoma kinases (ALK). For example, alkylation of 4-CF3OC6H4OH with tert-Bu bromoacetate followed by treatment with TFA and chlorination with SOCl2 gave an acyl chloride (97% yield for three steps), which underwent amidation with amine II (preparation given) to afford amide III. This compds. showed inhibition against ALK with IC50 < 50 nM in the luciferase-coupled chemiluminescent kinase assay. Therefore, I and their pharmaceutical compns. are useful for modulating protein kinase enzymic activity and for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion.

IT 867340-11-2P 867340-46-3P 867340-50-9P
867340-98-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(modulator; preparation of thiazoles and analogs as anaplastic lymphoma kinase modulators)

RN 867340-11-2 CAPLUS
CN 4-Thiazolecarboxamide, N-[2-(3-chlorophenyl)ethyl]-2-[[[2-[4-(trifluoromethoxy)phenoxy]acetyl]amino]methyl]- (CA INDEX NAME)

PAGE 1-A



L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

RN 867340-46-3 CAPLUS
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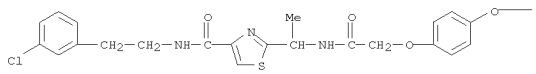
PAGE 1-A



PAGE 1-B

RN 867340-50-9 CAPLUS
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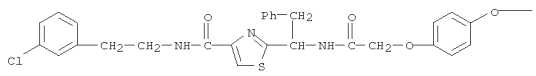
PAGE 1-A

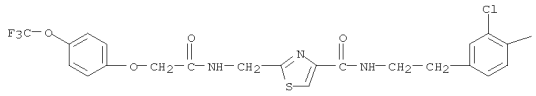


PAGE 1-B

RN 867340-98-5 CAPLUS
CN 4-Thiazolecarboxamide, N-[2-(3,4-dichlorophenyl)ethyl]-2-[[[2-[4-(trifluoromethoxy)phenoxy]acetyl]amino]methyl]- (CA INDEX NAME)

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> fil reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                             ENTRY    SESSION
FULL ESTIMATED COST                                           6.31     200.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)              SINCE FILE      TOTAL
                                                             ENTRY    SESSION
CA SUBSCRIBER PRICE                                          -0.85      -0.85

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STRUCTURE FILE UPDATES:   18 AUG 2010  HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES:  18 AUG 2010  HIGHEST RN 1236611-52-1

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http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\STNEXP\Queries\10598911.str
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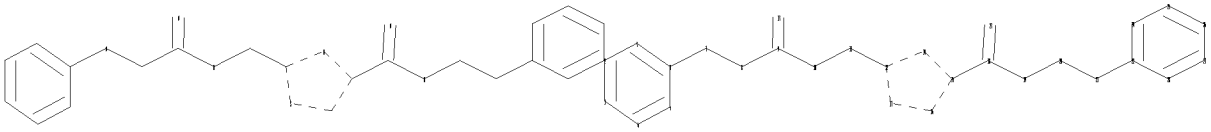

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chain nodes :
7  8  9  10  11  13  18  19  20  21  23
ring nodes :
1  2  3  4  5  6  12  14  15  16  17  22  24  25  26  27  28
chain bonds :
4-7  7-8  8-9  9-10  9-13  10-11  11-12  15-18  18-19  18-23  19-20  20-21  21-22
```

```
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  12-14  12-17  14-15  15-16  16-17  22-24  22-28
24-25  25-26  26-27  27-28
exact/norm bonds :
4-7  7-8  9-10  9-13  10-11  12-14  12-17  14-15  15-16  16-17  18-19  18-23  19-20

exact bonds :
8-9  11-12  15-18  20-21  21-22
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  22-24  22-28  24-25  25-26  26-27  27-28


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
 11:CLASS  12:Atom  13:CLASS  14:Atom  15:Atom  16:Atom  17:Atom  18:CLASS
19:CLASS  20:CLASS  21:CLASS  22:Atom  23:CLASS  24:Atom  25:Atom  26:Atom  27:Atom
 28:Atom




L5      STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5              STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l5
SAMPLE SEARCH INITIATED 15:01:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        5 TO ITERATE

100.0% PROCESSED        5 ITERATIONS                                 4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            5 TO      234
PROJECTED ANSWERS:               4 TO      200

L6            4 SEA SSS SAM L5

=> s l5 ful
FULL SEARCH INITIATED 15:01:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       96 TO ITERATE

100.0% PROCESSED       96 ITERATIONS                                52 ANSWERS
SEARCH TIME: 00.00.01

L7           52 SEA SSS FUL L5

=> fil caplus
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
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	ENTRY	SESSION
FULL ESTIMATED COST	198.89	399.82

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.85

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FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010 (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l7
L8 1 L7

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.50	400.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.85

FILE 'REGISTRY' ENTERED AT 15:01:43 ON 19 AUG 2010
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STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

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predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
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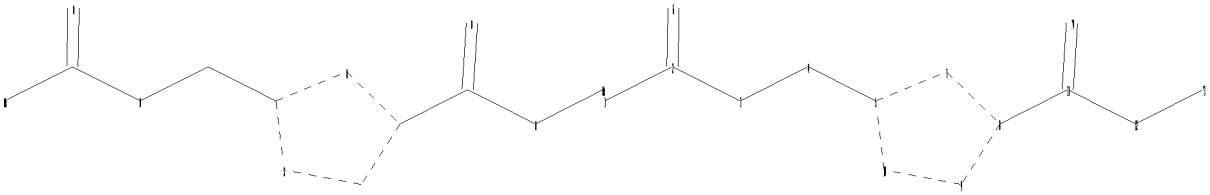
=>
Uploading C:\Program Files\STNEXP\Queries\10598911b.str



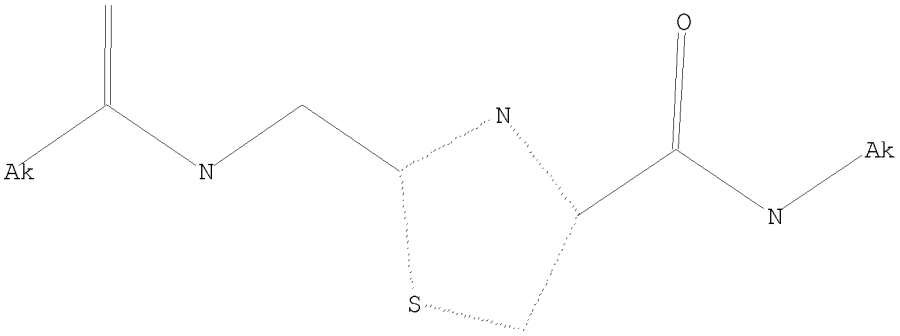
chain nodes :
1 2 3 4 6 11 12 13 14
ring nodes :
5 7 8 9 10
chain bonds :
1-2 2-3 2-6 3-4 4-5 8-11 11-12 11-14 12-13
ring bonds :
5-7 5-10 7-8 8-9 9-10
exact/norm bonds :
1-2 2-3 2-6 3-4 5-7 5-10 7-8 8-9 9-10 11-12 11-14 12-13
exact bonds :
4-5 8-11

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS

L9   STRUCTURE UPLOADED

=> d
L9 HAS NO ANSWERS

L9 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s l9
SAMPLE SEARCH INITIATED 15:04:30 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      507 TO ITERATE

100.0% PROCESSED      507 ITERATIONS                              50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         8790 TO    11490
PROJECTED ANSWERS:             592 TO     1448

L10          50 SEA SSS SAM L9

=> s l9 ful
FULL SEARCH INITIATED 15:04:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     9877 TO ITERATE

100.0% PROCESSED     9877 ITERATIONS                          1053 ANSWERS
SEARCH TIME: 00.00.01

L11        1053 SEA SSS FUL L9

=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   193.50     593.82

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -0.85

FILE 'CAPLUS' ENTERED AT 15:04:36 ON 19 AUG 2010
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FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010 (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
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This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l11
L12   217 L11

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.50	594.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.85

FILE 'REGISTRY' ENTERED AT 15:04:41 ON 19 AUG 2010

Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
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experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> fil reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 1.47 | 595.79

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | 0.00 | -0.85

FILE 'REGISTRY' ENTERED AT 15:06:40 ON 19 AUG 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
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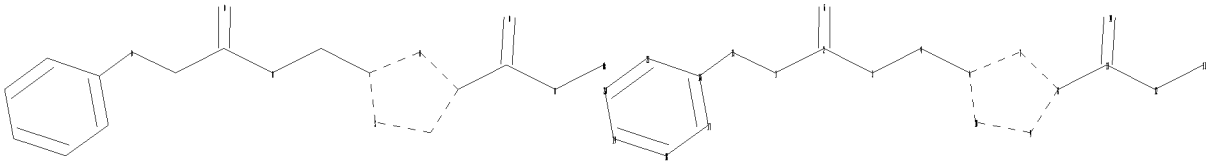

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1  2  3  4  6  11  12  13  14  15
ring nodes :
5  7  8  9  10  16  17  18  19  20  21
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ring bonds :
5-7  5-10  7-8  8-9  9-10  16-17  16-21  17-18  18-19  19-20  20-21
exact/norm bonds :
1-15  2-3  2-6  3-4  5-7  5-10  7-8  8-9  9-10  11-12  11-14  12-13  15-16
exact bonds :
1-2  4-5  8-11
normalized bonds :
16-17  16-21  17-18  18-19  19-20  20-21


Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:Atom  6:CLASS  7:Atom  8:Atom  9:Atom
10:Atom  11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:Atom  17:Atom
18:Atom  19:Atom  20:Atom  21:Atom



L13     STRUCTURE UPLOADED

=> d
L13 HAS NO ANSWERS
L13             STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


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SAMPLE SEARCH INITIATED 15:06:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       52 TO ITERATE

100.0% PROCESSED       52 ITERATIONS                              15 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          608 TO     1472
PROJECTED ANSWERS:              68 TO      532

L14          15 SEA SSS SAM L13

=> s l13 ful
FULL SEARCH INITIATED 15:07:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1069 TO ITERATE

100.0% PROCESSED     1069 ITERATIONS                            203 ANSWERS
SEARCH TIME: 00.00.01

L15         203 SEA SSS FUL L13
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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     191.54     787.33

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                       0.00      -0.85

FILE 'CAPLUS' ENTERED AT 15:07:03 ON 19 AUG 2010
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FILE COVERS 1907 - 19 Aug 2010  VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010  (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Jun 2010

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

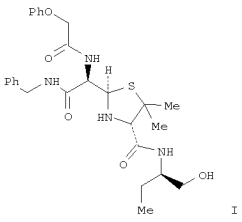
http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l15
L16          5 L15

=> d ibib abs hitstr tot
```

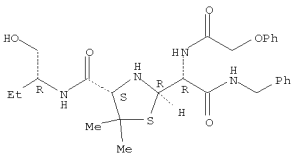
L16 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2006:128442 CAPLUS
DOCUMENT NUMBER: 144:369954
TITLE: Stereoselective synthesis of a thiazolane amide using molecular recognition in the triazolyl-activated ester intermediate
AUTHOR(S): Styring, Peter; Chong, Sannie S. F.
CORPORATE SOURCE: Department of Chemical and Process Engineering, The University of Sheffield, Sheffield, S1 3JD, UK
SOURCE: Tetrahedron Letters (2006), 47(11), 1737-1740
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:369954
GI



I

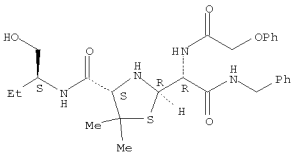
AB Amide I, derived from penicillin V and racemic (R/S)-2-aminobutanol, was prepared with 83% de and shows significantly higher toxicity than the pure diastereomers prepared from homochiral 2-aminobutanol. This has been attributed to conformational changes in the resolved product brought about through hydrogen-bonded self-assembly in the intermediate. The data generally indicated that a min. concentration of 68 μg/mL was required to impart a toxicol. effect to 50% of the cultured cell, or 104 μg/mL for 90% of the cultured cell. This gave a pos. implication stating that the above final compds. were relatively 'safe' and should proceed to the next stage of testing to determine their anti-viral potential.
IT 881854-48-4P 881854-56-4P
RL: ADV (Adverse effect, including toxicity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective synthesis of a thiazolane amide using mol. recognition in the triazolyl-activated ester intermediate)
RN 881854-48-4 CAPLUS
CN 2-Thiazolidineacetamide, 4-[[[(1R)-1-(hydroxymethyl)propyl]amino]carbonyl]-5,5-dimethyl-α-[(2-phenoxyacetyl)amino]-N-(phenylmethyl)-, (αR,2R,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 881854-56-4 CAPLUS
CN 2-Thiazolidineacetamide, 4-[[[(1S)-1-(hydroxymethyl)propyl]amino]carbonyl]-5,5-dimethyl-α-[(2-phenoxyacetyl)amino]-N-(phenylmethyl)-, (αR,2R,4S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1126676 CAPLUS
DOCUMENT NUMBER: 143:405899
TITLE: Preparation of thiazoles and analogs as anaplastic lymphoma kinase modulators
INVENTOR(S): Leahy, James William; Lewis, Gary Lee; Nuss, John M.; Ridgway, Brian Hugh; Sangalang, Joan C.
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 346 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005097765	A1	20051020	WO 2005-US10969	20050331
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005230847	A1	20051020	AU 2005-230847	20050331
CA 2559866	A1	20051020	CA 2005-2559866	20050331
EP 1730128	A1	20061213	EP 2005-733275	20050331
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2008502595	T	20080131	JP 2007-506579	20050331
US 20090186905	A1	20090723	US 2007-598911	20070607
PRIORITY APPLN. INFO.:			US 2004-558800P P	20040331
			WO 2005-US10969 W	20050331

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 143:405899; MARPAT 143:405899
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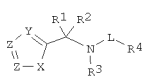

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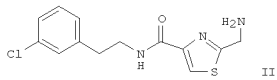

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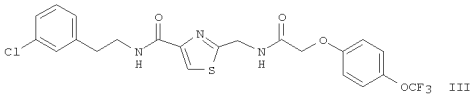

III

AB Title compds. I [wherein R1, R2 = H, halo, trihalomethyl; R1 and R2 are oxo; R3, R4 = H, (un)substituted alkyl, aryl; X = O, S; Y = (un)substituted CH or N; one of Z = C(COO-alkyl), C(CONH-alkyl), while the other Z = N, (un)substituted CH; L = C(O/S), SO2 or absence; etc., pharmaceutically acceptable salts, hydrates or prodrugs thereof] as modulators of protein kinases, especially anaplastic lymphoma kinases (ALK).
For example, alkylation of 4-CF3OC6H4OH with tert-Bu bromoacetate followed by treatment with TFA and chlorination with SOCl2 gave an acyl chloride (97% yield for three steps), which underwent amidation with amine II (preparation given) to afford amide III. This compds. showed inhibition against ALK with IC50 < 50 nM in the luciferase-coupled chemiluminescent kinase assay. Therefore, I and their pharmaceutical compns. are useful for modulating protein kinase enzymic activity and for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion.
IT 867340-11-2P 867340-14-5P 867340-17-8P
867340-20-3P 867340-46-3P 867340-50-9P
867340-56-5P 867340-63-4P 867340-65-6P
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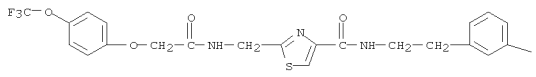
867343-62-2P 867343-65-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(modulator; prepn. of thiazoles and analogs as anaplastic lymphoma kinase modulators)

RN 867340-11-2 CAPLUS
CN 4-Thiazolecarboxamide, N-[2-(3-chlorophenyl)ethyl]-2-[[[2-[4-(trifluoromethoxy)phenoxy]acetyl]amino]methyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

RN 867340-14-5 CAPLUS
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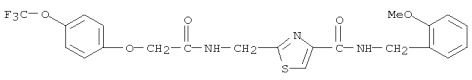

RN 867340-17-8 CAPLUS
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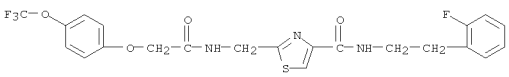

RN 867340-20-3 CAPLUS
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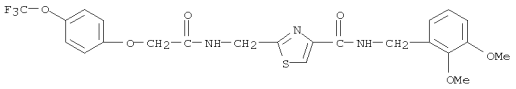

RN 867340-46-3 CAPLUS
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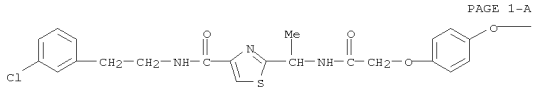
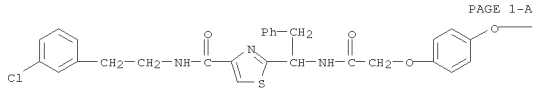
PAGE 1-A



PAGE 1-B

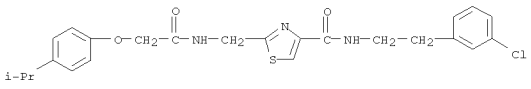
RN 867340-50-9 CAPLUS
CN 4-Thiazolecarboxamide, N-[2-(3-chlorophenyl)ethyl]-2-[2-phenyl-1-[[2-[4-(trifluoromethoxy)phenoxy]acetyl]amino]ethyl]- (CA INDEX NAME)

PAGE 1-A



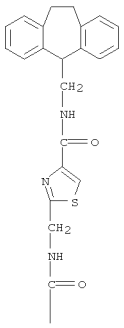
PAGE 1-B

RN 867340-56-5 CAPLUS
CN 4-Thiazolecarboxamide, N-[2-(3-chlorophenyl)ethyl]-2-[[[2-[4-(1-methylethyl)phenoxy]acetyl]amino]methyl]- (CA INDEX NAME)



RN 867340-63-4 CAPLUS
CN 4-Thiazolecarboxamide, N-[(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)methyl]-2-[[[2-[4-(trifluoromethoxy)phenoxy]acetyl]amino]methyl]- (CA INDEX NAME)

PAGE 1-A



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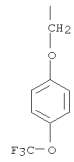
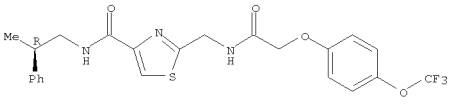


RN 867340-65-6 CAPLUS
CN 4-Thiazolecarboxamide, N-[(2R)-2-phenylpropyl]-2-[[[2-[4-(trifluoromethoxy)phenoxy]acetyl]amino]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



L16 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1993:191729 CAPLUS
DOCUMENT NUMBER: 118:191729
ORIGINAL REFERENCE NO.: 118:32941a,32944a
TITLE: Preparation of bis(carbamoylthiazolidine) derivatives as virucides
INVENTOR(S): Humber, Dai Cedric; Weingarten, Gordon Gad; Storer, Richard; Kitchin, John; Hann, Michael Menteith
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9220665	A1	19921126	WO 1992-GB840	19920508
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG				
AU 9217450	A	19921230	AU 1992-17450	19920508
PRIORITY APPLN. INFO.:			GB 1991-10093	A 19910510
			GB 1991-12481	A 19910611
			WO 1992-GB840	A 19920508

OTHER SOURCE(S): MARPAT 118:191729
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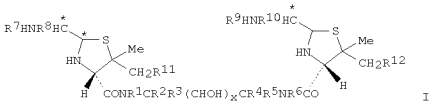
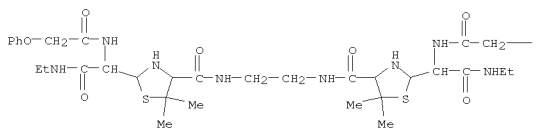


I

AB Title compds. [I; x = 0-2; R1, R6 = H, (hydroxy)alkyl; R2, R3, R4, R5 = H, Me, Et, CH2OH, CH2NH2, CO2H; R7, R9 = H, alkyl, cycloalkyl, aralkyl, arylcarbonyl, COCH:CHPh, SO2CH:CHPh, arylsulfonyl, phenylcycloalkylcarbonyl, SO2CH:CHPh, etc.; R8, R10 = H, alkyl, CO2H, alkoxycarbonyl, aralkoxycarbonyl, carbamoyl, cycloalkyl, cycloalkylalkyl, aminoalkyl etc.; R11, R12 = H, OH, AcO; starred atoms are (R)-configuration], were prepared Thus, ClCO2Et was stirred with benzylpenicillin N-ethylpiperidine salt in CHCl3 at -11° for 2 h; H2NCH2CH2NH2 was added at <0° and the mixture was stirred 2 h and allowed to reach room temperature to give [2(S)-[2α,5α,6β]]-N,N'-[1,2-ethanediylbis[3,3-dimethyl-7-oxo-6-[(phenylacetyl)amino]-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxamide. This was stirred with EtNH2 in CH2Cl2 to give [2(R)-[2α(R*),4β]]-4,4'-[1,2-ethanediylbis[aminocarbonyl]bis[N-ethyl-5,5-dimethyl-α-[(phenylacetyl)amino]-2-

L16 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
thiazolidineacetamide]]. I inhibited HIV protease with EC50 ≤ 100 nM.
IT 146654-31-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as virucide)
RN 146654-31-1 CAPLUS
CN 2-Thiazolidineacetamide, 4,4'-[1,2-ethanediylbis(iminocarbonyl)]bis[N-ethyl-5,5-dimethyl-α-[(phenoxyacetyl)amino]-, [2R-[2α(R*),4β[2'R*(R*),4'S*]]]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— OPh

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1978:170068 CAPLUS
DOCUMENT NUMBER: 88:170068
ORIGINAL REFERENCE NO.: 88:26807a,26810a
TITLE: Application of 8-hydroxyquinoline in the synthesis of semi-synthetic β-lactam antibiotics and their esters
AUTHOR(S): Sztaricskai, Ferenc; Miskolczi, Istvan; R. Farkas, Erzsebet; Bognar, Rezso
CORPORATE SOURCE: Dep. Org. Chem., Lajos Kossuth Univ., Debrecen, Hung.
SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1977), 94(2), 169-76
CODEN: ACASA2; ISSN: 0001-5407
DOCUMENT TYPE: Journal
LANGUAGE: English
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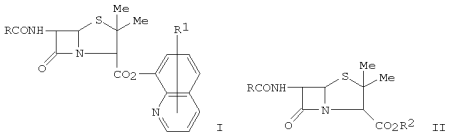
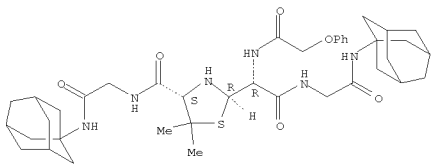


I II

AB Esters I [R = benzyl, PhOCH2, 5-methyl-3-phenyl-4-isoxazolyl, 2-thienylmethyl, 2,6-(MeO)2C6H3; R1 = H, 4-Me, 5-Ac, 5-Et, 5-NO, 6-Me] were prepared in 11.4-71% yield by reaction of the penicillin derivative with the resp. 8-quinolinol. I were effective in vitro against Mycobacterium tuberculosis H37Rv and other INH- and streptomycin-resistant tuberculosis strains. I were used for the synthesis of II (R = 2-thienylmethyl, ClCH2, R2 = H; R = 2-thienylmethyl, PhOCH2, R2 = CH2CCl3).
IT 66302-15-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 66302-15-6 CAPLUS
CN 2-Thiazolidineacetamide, 5,5-dimethyl-N-[2-oxo-2-(tricyclo[3.3.1.13,7]dec-1-ylamino)ethyl]-4-[[[2-oxo-2-(tricyclo[3.3.1.13,7]dec-1-ylamino)ethyl]amino]carbonyl]-α-[(2-phenoxyacetyl)amino]-, (αR,2R,4S)- (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



ACCESSION NUMBER: 1977:72508 CAPLUS
DOCUMENT NUMBER: 86:72508
ORIGINAL REFERENCE NO.: 86:11487a,11490a
TITLE: Modification of 6-aminopenicillanic acid derivatives
AUTHOR(S): Zukowski, Edward; Eckstein, Zygmunt
CORPORATE SOURCE: "Polfa" Res. Lab., Warsaw, Pol.
SOURCE: Polish Journal of Pharmacology and Pharmacy (1976), 28(4), 379-87
CODEN: PJPPAA; ISSN: 0301-0244
DOCUMENT TYPE: Journal
LANGUAGE: English
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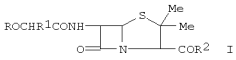

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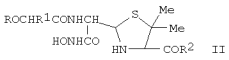
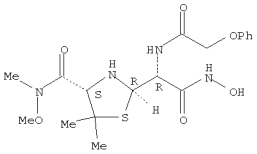


II

AB The penicillin esters and amides I (R = Ph, R1 = H, R2 = OMe, OCH2Ph, NEt2, cyclohexylamino, NHPh, NHC6H4Me-3, NHON+HEt3, NHOMe, NMeOMe; R = Ph, R1 = Me, R2 = NEt2, NHPh, NHON+HEt3, NHOH, NHOMe; R = 4-MeC6H4, R1 = H, R2 = NEt2, NHPh, NHC6H4Me-3; R = 2,4-MeClC6H3, R1 = Me, R2 = NHOMe) were prepared from the triethylamine, Na, or K salts by mixed anhydride method. II (R = Ph, R1 = H, R2 = OH, OMe, OCH2Ph, NHOMe, NMeOMe; R = Ph, R1 = Me, R2 = OH, NHOMe; R = 3,4-Cl2C6H3, 2,4,5-Cl3C6H2, R1 = H, R2 = OH; R = 3,4-MeClC6H3, R1 = Me, R2 = OH; R = 2,4-MeClC6H3, R1 = Me, R2 = NHOMe) were obtained by treating the triethylamine salts with NH2OH.HCl or NH2OMe.HCl.
IT 61700-40-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 61700-40-1 CAPLUS
CN 2-Thiazolidineacetamide, N-hydroxy-4-[(methoxymethylamino)carbonyl]-5,5-dimethyl-α-[(phenoxyacetyl)amino]-, [2R-[2α(R*),4β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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                                                         ENTRY    SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                      -4.25      -5.10

FILE 'REGISTRY' ENTERED AT 15:09:12 ON 19 AUG 2010
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STRUCTURE FILE UPDATES:   18 AUG 2010  HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES:  18 AUG 2010  HIGHEST RN 1236611-52-1

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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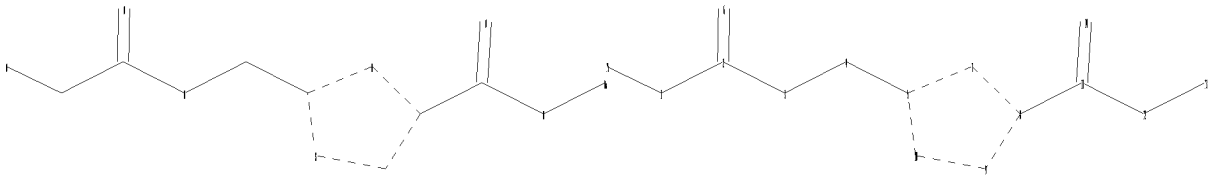

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ring nodes :
5  7  8  9  10
chain bonds :
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ring bonds :
5-7  5-10  7-8  8-9  9-10
exact/norm bonds :
```

1-15 2-3 2-6 3-4 5-7 5-10 7-8 8-9 9-10 11-12 11-14 12-13
exact bonds :
1-2 4-5 8-11

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L17   STRUCTURE UPLOADED

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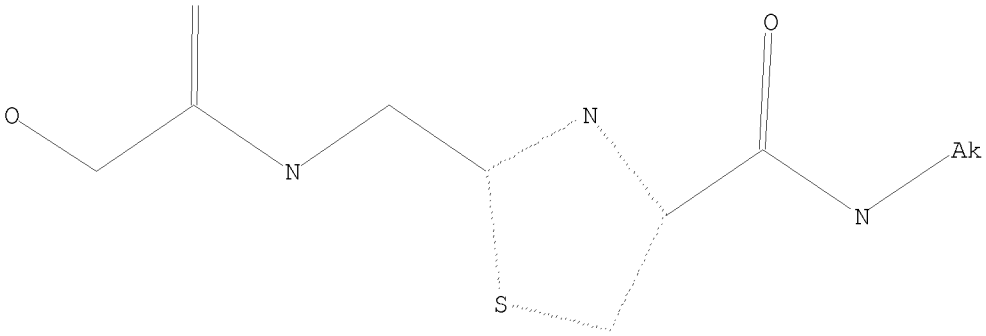
L17 HAS NO ANSWERS
L17   STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -   142 TO ITERATE

100.0% PROCESSED   142 ITERATIONS   15 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 2126 TO   3554
PROJECTED ANSWERS: 68 TO   532

L18   15 SEA SSS SAM L17

=> s l17 ful
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FULL SCREEN SEARCH COMPLETED -   3055 TO ITERATE

100.0% PROCESSED   3055 ITERATIONS   214 ANSWERS
SEARCH TIME: 00.00.01

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L19         214 SEA SSS FUL L17

=> fil caplus
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FULL ESTIMATED COST                                       191.54    1009.92

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)              SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                         0.00      -5.10

FILE 'CAPLUS' ENTERED AT 15:10:03 ON 19 AUG 2010
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FILE COVERS 1907 - 19 Aug 2010  VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010  (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Jun 2010

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

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L20           5 L19

=> fil reg
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                                                           ENTRY    SESSION
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CA SUBSCRIBER PRICE                                         0.00      -5.10

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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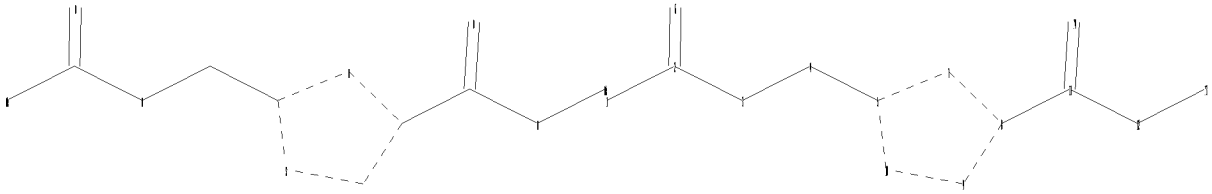

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ring nodes :
5 7 8 9 10
chain bonds :
1-2 2-3 2-6 3-4 4-5 8-11 11-12 11-14 12-13
ring bonds :
5-7 5-10 7-8 8-9 9-10
exact/norm bonds :
1-2 2-3 2-6 3-4 5-7 5-10 7-8 8-9 9-10 11-12 11-14 12-13
exact bonds :
4-5 8-11

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS

L21 STRUCTURE UPLOADED

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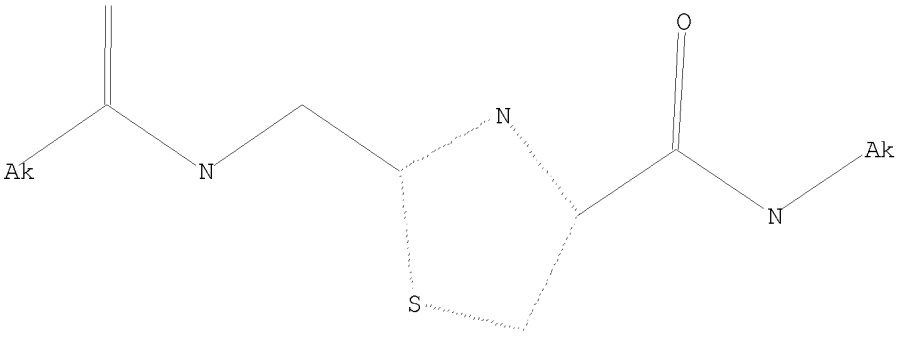
L21 HAS NO ANSWERS
L21 STR



Structure attributes must be viewed using STN Express query preparation.

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INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
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FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
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PROJECTED ANSWERS: 592 TO 1448

L22 50 SEA SSS SAM L21

=> s l21 ful
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100.0% PROCESSED 9877 ITERATIONS 1053 ANSWERS
SEARCH TIME: 00.00.01

L23 1053 SEA SSS FUL L21

=> fil caplus
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CA SUBSCRIBER PRICE 0.00 -5.10

FILE 'CAPLUS' ENTERED AT 15:12:32 ON 19 AUG 2010

FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010 (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2010.

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http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

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L24        217 L23

=> s l24 and thiazole
          21400 THIAZOLE
           5238 THIAZOLES
          23369 THIAZOLE
                  (THIAZOLE OR THIAZOLES)
L25          63 L24 AND THIAZOLE

=> s l25 and carboxamide
          21373 CARBOXAMIDE
           5584 CARBOXAMIDES
          24330 CARBOXAMIDE
                  (CARBOXAMIDE OR CARBOXAMIDES)
L26           4 L25 AND CARBOXAMIDE

=> d ibib abs hitstr tot
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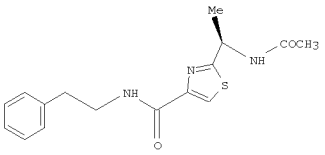
L26 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:430528 CAPLUS
DOCUMENT NUMBER: 151:3563
TITLE: Neobacillamide A, a novel thiazole -containing alkaloid from the marine bacterium Bacillus vallismortis C89, associated with South China Sea sponge Dysidea avara
AUTHOR(S): Yu, Lu-Lu; Li, Zhen-Yu; Peng, Chong-Sheng; Li, Zhi-Yong; Guo, Yue-Wei
CORPORATE SOURCE: Key Laboratory of Microbial Metabolism, School of Life Science and Biotechnology, Ministry of Education, China, Shanghai Jiao Tong University, Shanghai, 200240, Peop. Rep. China
SOURCE: Helvetica Chimica Acta (2009), 92(3), 607-612
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



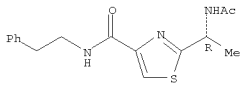
I

AB A novel thiazole alkaloid, neobacillamide A (I), together with a known related one, bacillamide C, was isolated from the bacterium Bacillus vallismortis C89, associated with the South China Sea sponge Dysidea avara. The structure of I was elucidated on the basis of its spectroscopic data. A plausible biosynthetic pathway is proposed. I represents the first example of a thiazole-carboxamide bearing a 2-phenylethylamine moiety.

IT 1158821-83-0P
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(neobacillamide A as thiazole-containing alkaloid from marine Bacillus vallismortis with sponge Dysidea avara)
RN 1158821-83-0 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-(2-phenylethyl)- (CA INDEX NAME)

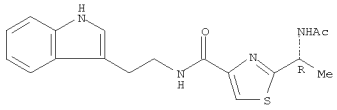
Absolute stereochemistry. Rotation (-).

L26 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



IT 959853-22-6P
RL: BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(neobacillamide A as thiazole-containing alkaloid from marine Bacillus vallismortis with sponge Dysidea avara)
RN 959853-22-6 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-[2-(1H-indol-3-yl)ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2006:916886 CAPLUS
DOCUMENT NUMBER: 145:314980
TITLE: Preparation of aminopyridine compounds with spleen tyrosine kinase (Syk)-inhibitory activity
INVENTOR(S): Kodama, Yoshitoshi; Noji, Satoru; Imamura, Katsuaki; Mizojiri, Ryo; Aoki, Kenta; Takagi, Hideo; Naka, Yuichi; Ito, Goro; Shinoda, Kiyotaka; Fujiwara, Akihito; Kurihara, Kazunori; Tanaka, Masaru
PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
SOURCE: PCT Int. Appl., 467pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006093247	A1	20060908	WO 2006-JP304034	20060224
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2006219231	A1	20060908	AU 2006-219231	20060224
AU 2006219231	B2	20100114		
CA 2599544	A1	20060908	CA 2006-2599544	20060224
EP 1854793	A1	20071114	EP 2006-728596	20060224
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
BR 2006007062	A2	20090804	BR 2006-7062	20060224
RU 2363699	C2	20090810	RU 2007-135872	20060224
ZA 2007007227	A	20090826	ZA 2007-7227	20060224
NZ 561000	A	20100129	NZ 2006-561000	20060224
US 20060205731	A1	20060914	US 2006-363563	20060228
MX 2007010459	A	20071011	MX 2007-10459	20070827
KR 2007099047	A	20071008	KR 2007-719698	20070828
KR 917511	B1	20090916		
IN 2007CN03771	A	20071123	IN 2007-CN3771	20070828
CN 101166734	A	20080423	CN 2006-80012848	20071017
PRIORITY APPLN. INFO.:			JP 2005-52469 A	20050228
			US 2005-658885P P	20050304
			JP 2006-11751 A	20060119
			US 2006-763045P P	20060127
			WO 2006-JP304034 W	20060224

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

L26 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 145:314980
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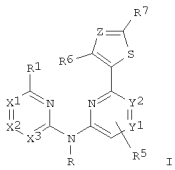


I

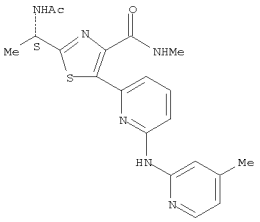
AB The title compds. [I; X1, X2, X3 = N, (un)saturated CH; Y1, Y2 = CH, N; R = H, C1-6 alkyl, acyl; R5 = H, C1-6 alkyl optionally substituted by HO or C1-6 alkoxy, CO2H, C1-6 alkoxycarbonyl, NO2; R6 = H, C1-6 alkyl optionally substituted by HO or C1-6 alkoxy, CO2H, C1-6 alkoxycarbonyl, each (un)substituted NH2 or CONH2, acyl; R7 = H, halo, NO2, cyano, each (un)substituted hydroxyalkyl or aminoalkyl, five-membered or six-membered saturated heterocyclic group, aromatic heterocyclic group, etc.] or salts thereof are prepared These compds. not only have high Syk inhibitory activity but also selectively inhibit Syk. They are useful for the treatment and/or prevention of allergic diseases, bronchial asthma, allergic rhinitis, allergic dermatitis, allergic conjunctivitis, or autoimmune diseases and for the treatment of articular rheumatism, systemic lupus erythematosus, multiple sclerosis, malignant tumor (in particular B lymphoma and B cell leukemia). Thus, 2-bromo-6-chloromethylpyridine and 2-thiocarbamoylpiperidine-4-carboxylic acid Et ester were heated in ethanol under refluxing for 2 h and the resulting mixture was cooled to room temperature, treated with DMF di-Me acetal and Et3N, and refluxed for 1 h to give 1-[5-(6-bromopyridin-2-yl)thiazol-2-yl]piperidine-4-carboxylic acid Et ester (II). II underwent amination with amination with 2-amino-4-picoline in the presence of rac-2,2'-bis(diphenylphosphino)-1,1'-binaphthyl, palladium acetate, and Cs2CO3 in toluene at 100° overnight to give 1-[5-[6-[(4-Methylpyridin-2-yl)amino]pyridin-2-yl]thiazol-2-yl]piperidine-4-carboxylic acid Et ester which was stirred with LiOH in aqueous methanol at 50° for 5 h, concentrated, and acidified with 0.1 N aqueous HCl solution to give 1-[5-[6-[(4-Methylpyridin-2-yl)amino]pyridin-2-yl]thiazol-2-yl]piperidine-4-carboxylic acid (III). III showed IC50 of ≤0.1 M μg/mL against.

IT 909284-40-8P 909284-47-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(prepn. of aminopyridine compds. as spleen tyrosine kinase (Syk) inhibitors for treatment and/or prevention of allergic diseases)

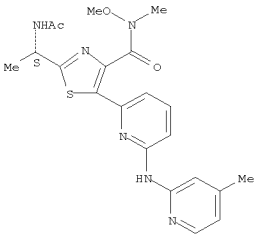
RN 909284-40-8 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1S)-1-(acetylamino)ethyl]-N-methyl-5-[6-[(4-methyl-2-pyridinyl)amino]-2-pyridinyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 909284-47-5 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1S)-1-(acetylamino)ethyl]-N-methoxy-N-methyl-5-[6-[(4-methyl-2-pyridinyl)amino]-2-pyridinyl]- (CA INDEX NAME)

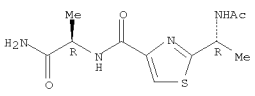
Absolute stereochemistry.



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

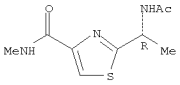
ACCESSION NUMBER: 1999:219066 CAPLUS
DOCUMENT NUMBER: 130:312089
TITLE: Ab initio calculations on peptide-derived oxazoles and thiazoles: improved molecular mechanics parameters for the AMBER force field
AUTHOR(S): Boden, Christopher D. J.; Pattenden, Gerald
CORPORATE SOURCE: Department of Chemistry, Nottingham University, Nottingham, NG7 2RD, UK
SOURCE: Journal of Computer-Aided Molecular Design (1999), 13(2), 153-166
CODEN: JCADEQ; ISSN: 0920-654X
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Ab initio calcns. at the RHF/6-31G* and MP2/6-31G*//RHF/6-31G* levels of theory are performed for 2-methyl-4-carboxamido-oxazoles and -thiazoles, including rotational profiles for the ring-carboxamide bond, which showed the expected conjugation and hydrogen bonding effects. On the basis of these data, newly optimized stretch, bend and torsional parameters for the AMBER* force field are derived, along with CHELPG-fitted partial atomic charges.
IT 223680-45-3 223680-49-7
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(ab initio calcns. on peptide-derived oxazoles and thiazoles)
RN 223680-45-3 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-[(1R)-2-amino-1-methyl-2-oxoethyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 223680-49-7 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



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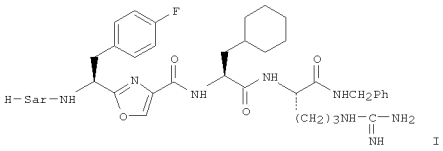
L26 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1998:482687 CAPLUS
DOCUMENT NUMBER: 129:231006
ORIGINAL REFERENCE NO.: 129:47015a
TITLE: Thrombin receptor (PAR-1) antagonists. Heterocycle-based peptidomimetics of the SFLLR agonist motif
AUTHOR(S): Hoekstra, William J.; Hulshizer, Becky L.; Mccomsey, David F.; Andrade-Gordon, Patricia; Kauffman, Jack A.; Addo, Michael F.; Oksenberg, Donna; Scarborough, Robert M.; Maryanoff, Bruce E.
CORPORATE SOURCE: The R. W. Johnson Pharmaceutical Research Institute, Spring House, PA, 19477, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1998), 8(13), 1649-1654
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



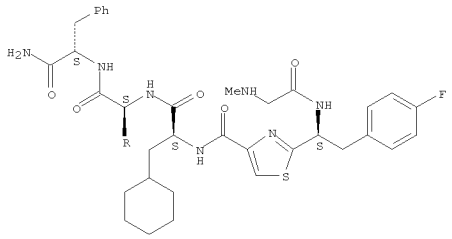
AB The thrombin receptor (PAR-1) is activated by α-thrombin to stimulate various cell types, including platelets, through the tethered-ligand sequence SFLLRN. A series of oxazole- or thiazole-based carboxamides, designed after SFLLR, were synthesized and evaluated in vitro. The compds. inhibited platelet aggregation induced by SFLLRN-NH2 or α-thrombin, and blocked the binding of [3H]-Ser-(p-F-Phe)-Har-Leu-Har-Lys-Tyr-NH2 (Har = homoarginine) to a CHRF membrane preparation of PAR-1. Oxazole-based peptide I bound to PAR-1 with an IC50 of 1.6 μM, and gave IC50 values of 25 μM and 6.6 μM against α-thrombin- and SFLLRN-NH2-induced platelet aggregation, resp.

IT 212756-41-7P 212756-47-3P 212756-48-4P
212756-49-5P 212756-50-8P 212756-53-1P
212756-54-2P 212756-55-3P 212756-56-4P
212756-57-5P 212756-58-6P 212756-59-7P
212756-60-0P 212756-61-1P 212756-62-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of oxazole- and thiazole-based peptidomimetics as thrombin receptor antagonists)

L26 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RN 212756-48-4 CAPLUS
CN L-Phenylalaninamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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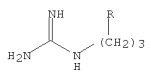
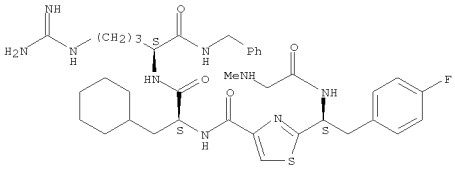


RN 212756-49-5 CAPLUS
CN L-Phenylalaninamide, L-valyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L26 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RN 212756-41-7 CAPLUS
CN L-Argininamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

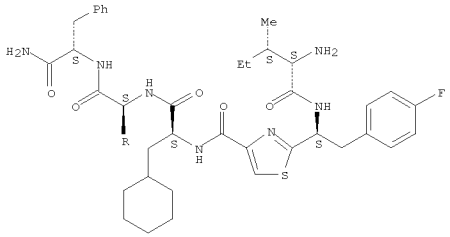
Absolute stereochemistry.



RN 212756-47-3 CAPLUS
CN L-Phenylalaninamide, L-isoleucyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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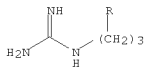
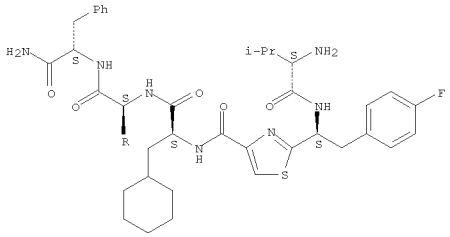


L26 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A



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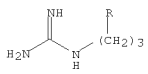
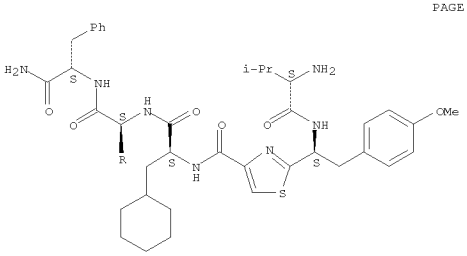
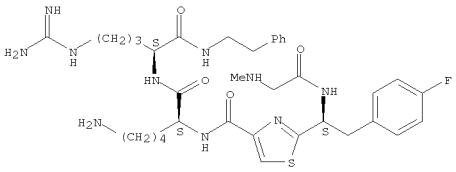


RN 212756-50-8 CAPLUS
CN L-Phenylalaninamide, L-valyl-2-[(1S)-1-amino-2-(4-methoxyphenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

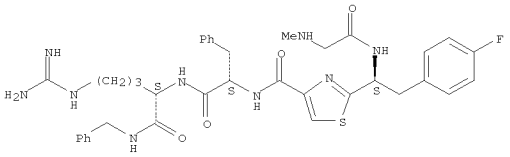
PAGE 1-A





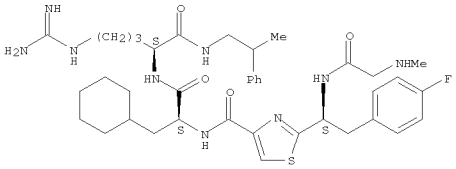
RN 212756-61-1 CAPLUS
CN L-Argininamide,
N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-L-phenylalanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 212756-62-2 CAPLUS
CN L-Argininamide,
N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-N-(2-phenylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

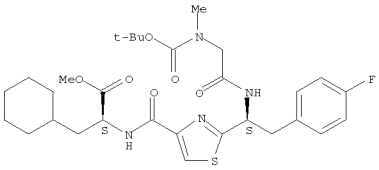


IT 212756-40-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of oxazole- and thiazole-based peptidomimetics as thrombin receptor antagonists)

L26 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 212756-40-6 CAPLUS
CN Cyclohexanepropanoic acid, α-[[[2-[(1S)-1-[[[[(1,1-dimethylethoxy)carbonyl]methylamino]acetyl]amino]-2-(4-fluorophenyl)ethyl]-4-thiazolyl]carbonyl]amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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CA SUBSCRIBER PRICE                                      -3.40      -8.50

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STRUCTURE FILE UPDATES:   18 AUG 2010  HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES:  18 AUG 2010  HIGHEST RN 1236611-52-1

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

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  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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STRUCTURE FILE UPDATES:   18 AUG 2010  HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES:  18 AUG 2010  HIGHEST RN 1236611-52-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.
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Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document. For information
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http://www.cas.org/support/stngen/stndoc/properties.html

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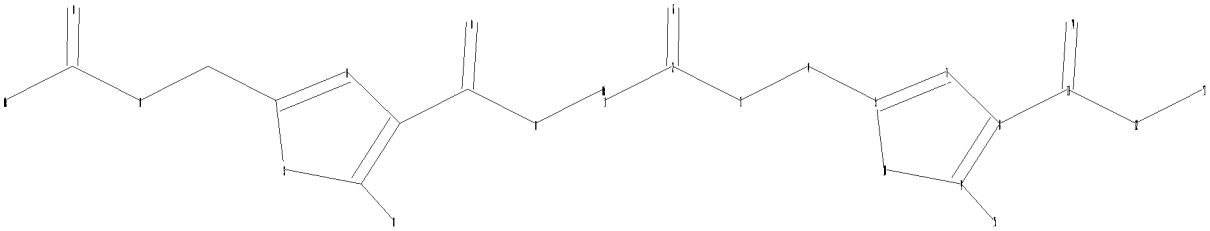

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exact/norm bonds :
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exact bonds :
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Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom
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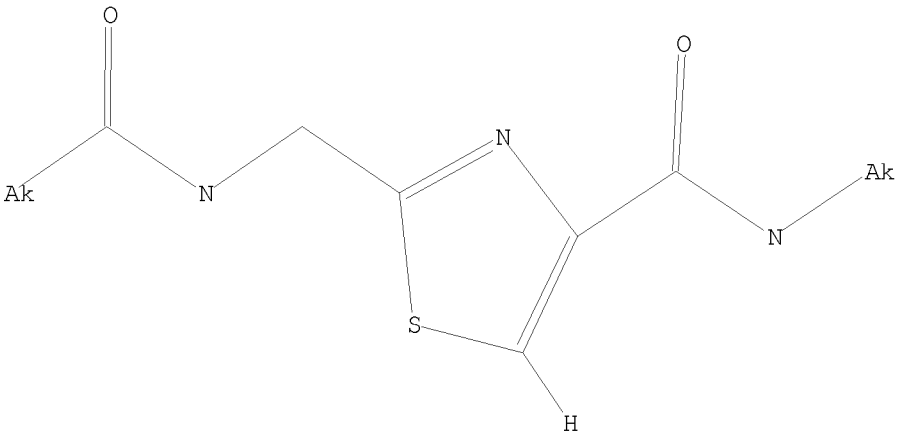

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L28          37 SEA SSS SAM L27

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CA SUBSCRIBER PRICE                                       0.00      -8.50

FILE 'CAPLUS' ENTERED AT 15:15:42 ON 19 AUG 2010
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FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010 (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2010.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

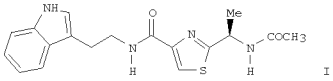
```
=> s l29
L30        151 L29

=> s l30 and thiazole
         21400 THIAZOLE
          5238 THIAZOLES
         23369 THIAZOLE
                 (THIAZOLE OR THIAZOLES)
L31         53 L30 AND THIAZOLE

=> d ibib abs hitstr tot
THE ESTIMATED COST FOR THIS REQUEST IS 307.93 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y
```

L31 ANSWER 1 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2010:74979 CAPLUS
DOCUMENT NUMBER: 152:357757
TITLE: (-)-Bacillamide C: the convergent approach
AUTHOR(S): Wang, Wei; Joyner, Shannon; Khoury, Kareem Andrew Sameer; Doemling, Alexander
CORPORATE SOURCE: Drug Discovery Institute, University of Pittsburgh, Pittsburgh, PA, 15261, USA
SOURCE: Organic & Biomolecular Chemistry (2010), 8(3), 529-532
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 152:357757
GI



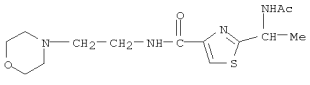
I

AB The newly discovered natural product bacillamide C (I) and several derivs. were convergently synthesized for the first time and in only three steps. The key transformation constitutes a thiazole Ugi multicomponent reaction. These compds. will serve to elucidate chemical biol. and SAR of this potent anti-algae natural product and shows the synthetic pathway to related natural products.

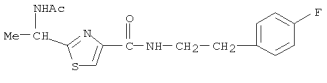
IT 1215381-42-2P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(cellular uptake of; preparation of bacillamide C derivs. via Ugi multicomponent reaction)

RN 1215381-42-2 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]ethyl]- (CA INDEX NAME)

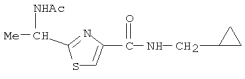
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)



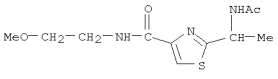
RN 1215381-34-2 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-[2-(4-fluorophenyl)ethyl]- (CA INDEX NAME)



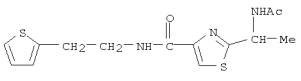
RN 1215381-35-3 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-(cyclopropylmethyl)- (CA INDEX NAME)



RN 1215381-36-4 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-(2-methoxyethyl)- (CA INDEX NAME)



RN 1215381-37-5 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



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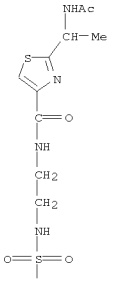

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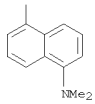
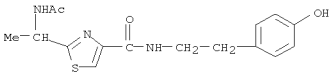


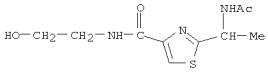
IT 1215381-23-9P 1215381-31-9P 1215381-34-2P
1215381-35-3P 1215381-36-4P 1215381-37-5P
1215381-39-7P 1215381-40-0P 1215381-44-4P
1215381-46-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of bacillamide C derivs. via Ugi multicomponent reaction)

RN 1215381-23-9 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-[2-(4-hydroxyphenyl)ethyl]- (CA INDEX NAME)

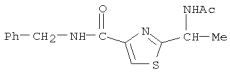


RN 1215381-31-9 CAPLUS

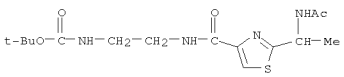
RN 1215381-39-7 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-(2-hydroxyethyl)- (CA INDEX NAME)



RN 1215381-40-0 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-(phenylmethyl)- (CA INDEX NAME)



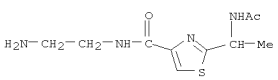
RN 1215381-44-4 CAPLUS
CN Carbamic acid, N-[2-[[[2-[1-(acetylamino)ethyl]-4-thiazolyl]carbonyl]amino]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 1215381-46-6 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-(2-aminoethyl)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 1215381-45-5
CMF C10 H16 N4 O2 S



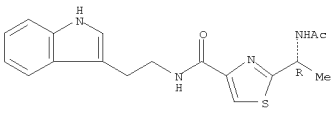
CM 2

CRN 76-05-1

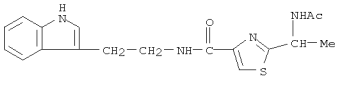
L31 ANSWER 1 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CMF C2 H F3 O2

IT 959853-22-6P, (-)-Bacillamide C 1020001-70-0P,
(±)-Bacillamide C
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of (-)-bacillamide C via Ugi multicomponent reaction using a
chiral auxiliary)
RN 959853-22-6 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-[2-(1H-indol-3-yl)ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 1020001-70-0 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-N-[2-(1H-indol-3-yl)ethyl]-
(CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
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REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:1405381 CAPLUS
DOCUMENT NUMBER: 152:185765
TITLE: Biosynthesis of indolocarbazole and goadsporin, two different heterocyclic antibiotics produced by actinomycetes
AUTHOR(S): Onaka, Hiroyasu
CORPORATE SOURCE: Department of Biotechnology, Faculty of Engineering and Biotechnology Research Center, Toyama Prefectural University, 5180 Kurokawa, Imizu, Toyama, 939-0398, Japan
SOURCE: Bioscience, Biotechnology, and Biochemistry (2009), 73(10), 2149-2155
CODEN: BBBIEJ; ISSN: 0916-8451
PUBLISHER: Japan Society for Bioscience, Biotechnology, and Agrochemistry
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. The biosynthesis of staurosporine, rebeccamycin, and goadsporin, which are produced by actinomycetes and contain characteristic
heterocyclic rings, was characterized by genetic methods. Staurosporine and rebeccamycin contain an indolocarbazole ring synthesized from two mols. of tryptophan, with indolepyruvic acid imine and chromopyrrolic acid
as biosynthetic intermediates. A tetrameric hemoprotein synthesizes chromopyrrolic acid, and cytochrome P 450 peroxidase catalyzes the intramol. C-C coupling and decarboxylation of chromopyrrolic acid to form the indolocarbazole core. Goadsporin is a thiopeptide containing thiazole and oxazole heterocyclic rings. The structural gene godA is ribosomally translated to a goadsporin precursor peptide, and oxazole, methyloxazole, and thiazole rings are derived from serine, threonine, and cysteine through post-translational modifications. On the basis of these knowledges, a wide variety of indolocarbazole and goadsporin analogs through the rational gene recombination and disruption of these biosynthetic genes were successfully produced.
IT 403476-91-5P, Goadsporin
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(biosynthesis of indolocarbazole and goadsporin, two different heterocyclic antibiotics produced by actinomycetes)
RN 403476-91-5 CAPLUS
CN L-Valine, N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbonyl]-

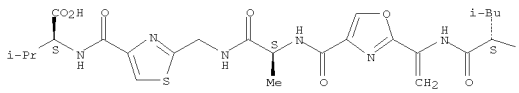
L-valyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-

1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L31 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A



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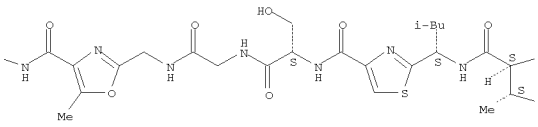

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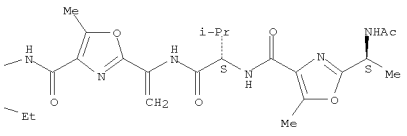

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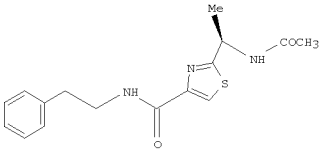
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:430528 CAPLUS
DOCUMENT NUMBER: 151:3563
TITLE: Neobacillamide A, a novel thiazole -containing alkaloid from the marine bacterium Bacillus vallismortis C89, associated with South China
Sea sponge Dysidea avara
AUTHOR(S): Yu, Lu-Lu; Li, Zhen-Yu; Peng, Chong-Sheng; Li, Zhi-Yong; Guo, Yue-Wei
CORPORATE SOURCE: Key Laboratory of Microbial Metabolism, School of Life
Science and Biotechnology, Ministry of Education, China, Shanghai Jiao Tong University, Shanghai, 200240, Peop. Rep. China
SOURCE: Helvetica Chimica Acta (2009), 92(3), 607-612
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

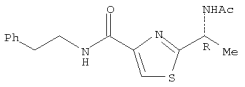


I

AB A novel thiazole alkaloid, neobacillamide A (I), together with a known related one, bacillamide C, was isolated from the bacterium Bacillus
vallismortis C89, associated with the South China Sea sponge Dysidea avara.
The structure of I was elucidated on the basis of its spectroscopic data. A plausible biosynthetic pathway is proposed. I represents the first example of a thiazole-carboxamide bearing a 2-phenylethylamine moiety.
IT 1158821-83-0P
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(neobacillamide A as thiazole-containing alkaloid from marine Bacillus vallismortis with sponge Dysidea avara)
RN 1158821-83-0 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-(2-phenylethyl)- (CA INDEX NAME)

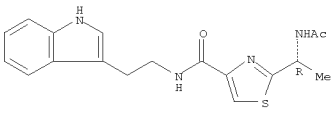
Absolute stereochemistry. Rotation (-).

L31 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



IT 959853-22-6P
RL: BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(neobacillamide A as thiazole-containing alkaloid from marine Bacillus vallismortis with sponge Dysidea avara)
RN 959853-22-6 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-[2-(1H-indol-3-yl)ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



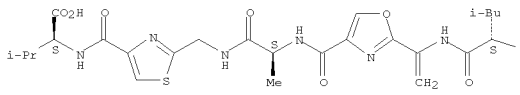
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 4 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:508320 CAPLUS
DOCUMENT NUMBER: 149:4947
TITLE: Discovery of a widely distributed toxin biosynthetic gene cluster
AUTHOR(S): Lee, Shaun W.; Mitchell, Douglas A.; Markley, Andrew L.; Hensler, Mary E.; Gonzalez, David; Wohlrab, Aaron; Dorrestein, Pieter C.; Nizet, Victor; Dixon, Jack E.
CORPORATE SOURCE: Department of Pharmacology, Department of Cellular and Molecular Medicine, Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2008), 105(15), 5879-5884
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bacteriocins represent a large family of ribosomally produced peptide antibiotics. Here we describe the discovery of a widely conserved biosynthetic gene cluster for the synthesis of thiazole and oxazole heterocycles on ribosomally produced peptides. These clusters encode a toxin precursor and all necessary proteins for toxin maturation and export. Using the toxin precursor peptide and heterocycle-forming synthetase proteins from the human pathogen Streptococcus pyogenes, we demonstrate the in vitro reconstitution of streptolysin S activity. We provide evidence that the synthetase enzymes, as predicted from our bioinformatics anal., introduce heterocycles onto precursor peptides, thereby providing mol. insight into the chemical structure of streptolysin S.
Furthermore, our studies reveal that the synthetase exhibits relaxed substrate specificity and modifies toxin precursors from both related and distant species. Given our findings, it is likely that the discovery of similar peptidic toxins will rapidly expand to existing and emerging genomes.
IT 403476-91-5P, Goadsporin
RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation)
(discovery of widely distributed toxin biosynthetic gene cluster)
RN 403476-91-5 CAPLUS
CN L-Valine, N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbonyl]-L-valyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L31 ANSWER 4 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A



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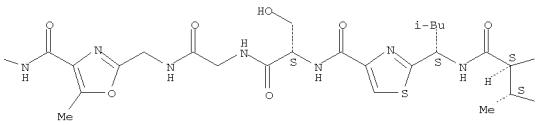

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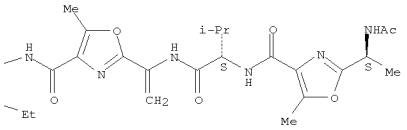

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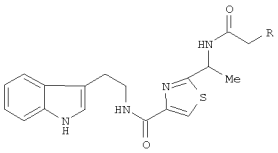
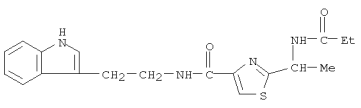
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 5 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:243207 CAPLUS
DOCUMENT NUMBER: 148:466583
TITLE: Tryptamine derived amides with thiazole ring system from Thermoactinomyces strain TA66-2
AUTHOR(S): Korkmaz, Cagla Akmemis; Hames-Kocabas, E. Esin; Uzel, Atac; Bedir, Erdal
CORPORATE SOURCE: Science Technology Center (EBILTEM), Ege University, Izmir, 35100, Turk.
SOURCE: Magnetic Resonance in Chemistry (2008), 46(1), 80-83
CODEN: MRCHEG; ISSN: 0749-1581
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



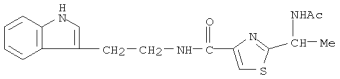
I R=Me
II R=H

AB A moderately thermophilic actinomycete strain, which was identified as Thermoactinomyces strain TA66-2, was isolated from hot-spring water. Fermentation, followed by solvent partition and chromatog. separation, resulted in the isolation of 2 new and 2 known mols. The structures of the new compds. were elucidated as 2-(1-propionylaminoethyl)thiazole-4-carboxylic acid [2-(1H-indol-3-yl)ethyl]amide (I) and 2-(1-acetylaminoethyl)thiazole-4-carboxylic acid [2-(1H-indol-3-yl)-ethyl]amide (II) by using spectral methods (1D- and 2D-NMR and LC-ESI-MS).
IT 1020001-66-4P 1020001-70-0P
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(tryptamine-derived amides with thiazole ring system from Thermoactinomyces)
RN 1020001-66-4 CAPLUS
CN 4-Thiazolecarboxamide, N-[2-(1H-indol-3-yl)ethyl]-2-[1-[(1-oxopropyl)amino]ethyl]- (CA INDEX NAME)



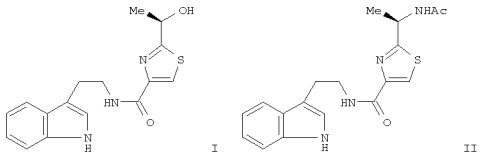
L31 ANSWER 5 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 1020001-70-0 CAPLUS
CN 4-Thiazolecarboxamide,
2-[1-(acetylamino)ethyl]-N-[2-(1H-indol-3-yl)ethyl]-
(CA INDEX NAME)



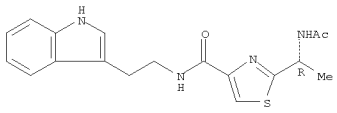
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 6 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2007:1288807 CAPLUS
DOCUMENT NUMBER: 148:49268
TITLE: Bacillamides from a hypersaline microbial mat bacterium
AUTHOR(S): Socha, Aaron M.; Long, Richard A.; Rowley, David C.
CORPORATE SOURCE: Department of Biomedical and Pharmaceutical Sciences, College of Pharmacy, University of Rhode Island, Kingston, RI, 02881, USA
SOURCE: Journal of Natural Products (2007), 70(11), 1793-1795
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society-American Society of Pharmacognosy
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Chemical studies of a Bacillus endophyticus isolated from a Bahamian hypersaline microbial mat led to the isolation of bacillamides B (I) and C (II), new tryptamide thiazole metabolites. Bioassay-guided fractionation using a HPLC-UV-MS bioassay technique enabled the detection of these trace fermentation products, and their total structures were elucidated by combined spectroscopic techniques.
IT 959853-22-6P, Bacillamide C
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(bacillamides from a hypersaline microbial mat bacterium)
RN 959853-22-6 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-[2-(1H-indol-3-yl)ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

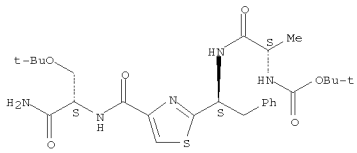


L31 ANSWER 6 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 7 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2007:442008 CAPLUS
DOCUMENT NUMBER: 147:73042
TITLE: Peptide-embedded heterocycles by mild single and multiple aza-Wittig ring closures
AUTHOR(S): Riedrich, Matthias; Harkal, Surendra; Arndt, Hans-Dieter
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Dortmund, Dortmund, 44221, Germany
SOURCE: Angewandte Chemie, International Edition (2007), 46(15), 2701-2703
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:73042
AB The aza-Wittig cyclization of amino acids and peptides is extremely mild, selective, and versatile. The reaction of amino acid esters and amino acid thioester azides delivered peptidic 1,3-azolines and 1,3-azoles with unsurpassed functional-group tolerance. This method allowed multiple ring closures and tolerates aqueous solvents.
IT 940951-17-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of thiazole-containing peptide via esterification of Boc-protected dipeptide with azido substituted dipeptide followed by aza-Wittig condensation)
RN 940951-17-7 CAPLUS
CN Carbamic acid, N-[(1S)-2-[[(1S)-1-[4-[[[(1S)-2-amino-1-[(1,1-dimethylethoxy)methyl]-2-oxoethyl]amino]carbonyl]-2-thiazolyl]-2-phenylethyl]amino]-1-methyl-2-oxoethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
(9 CITINGS)
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2006:17828 CAPLUS
DOCUMENT NUMBER: 144:426527
TITLE: Cloning and characterization of the goadsporin biosynthetic gene cluster from Streptomyces sp. TP-A0584
AUTHOR(S): Onaka, Hiroyasu; Nakaho, Mizuho; Hayashi, Keiko; Igarashi, Yasuhiro; Furumai, Tamotsu
CORPORATE SOURCE: Biotechnology Research Center, Toyama Prefectual University, Imizu, Toyama, 939-0398, Japan
SOURCE: Microbiology (Reading, United Kingdom) (2005), 151(12), 3923-3933
CODEN: MROBEO; ISSN: 1350-0872
PUBLISHER: Society for General Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

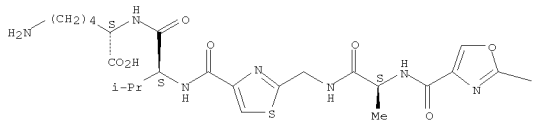
AB The biosynthetic gene cluster of goadsporin, a polypeptide antibiotic containing thiazole and oxazole rings, was cloned from Streptomyces sp. TP-A0584. The cluster contains a structural gene, godA, and nine god (goadsporin) genes involved in post-translational modification, immunity and transcriptional regulation. Although the gene organization is similar to typical bacteriocin biosynthetic gene clusters, each goadsporin biosynthetic gene shows low homol. to these genes. Goadsporin biosynthesis is initiated by the translation of godA, and the subsequent cyclization, dehydration and acetylation are probably catalyzed by godD, godE, godF, godG and godH gene products. GodI shows high similarity to the 54 kDa subunit of the signal recognition particle and plays an important role in goadsporin immunity. Furthermore, four goadsporin analogs were produced by site-directed mutagenesis of godA, suggesting that this biosynthesis machinery is used for the heterocyclization of peptides.

IT 884593-33-3P
RL: BPN (Biosynthetic preparation); PRP (Properties); BIOL (Biological study); PREP (Preparation)
(20K; cloning and characterization of goadsporin biosynthetic gene cluster from Streptomyces sp. TP-A0584)

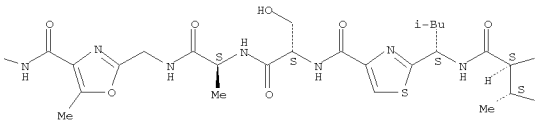
RN 884593-33-3 CAPLUS
CN L-Lysine,
N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbonyl]-
L-valyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-
1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

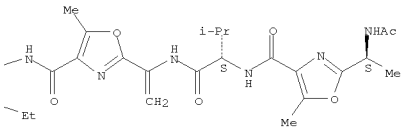
PAGE 1-A



PAGE 1-B



PAGE 1-C

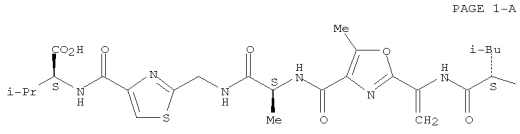


IT 884593-32-2P
RL: BPN (Biosynthetic preparation); PRP (Properties); BIOL (Biological study); PREP (Preparation)
(S15T; cloning and characterization of goadsporin biosynthetic gene cluster from Streptomyces sp. TP-A0584)

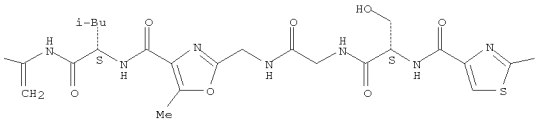
RN 884593-32-2 CAPLUS
CN L-Valine,
N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbonyl]-
L-valyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-
1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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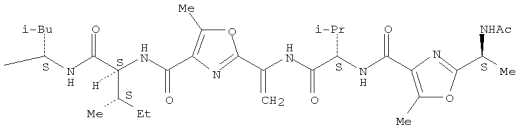
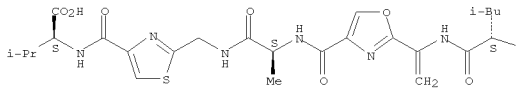


IT 884593-31-1P
RL: BPN (Biosynthetic preparation); PRP (Properties); BIOL (Biological study); PREP (Preparation)
(G10A; cloning and characterization of goadsporin biosynthetic gene cluster from Streptomyces sp. TP-A0584)

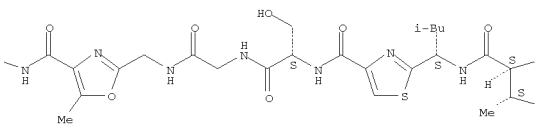
RN 884593-31-1 CAPLUS
CN L-Valine,
N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbonyl]-
L-valyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-
1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-seryl-L-alanyl-2-(aminomethyl)-
5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

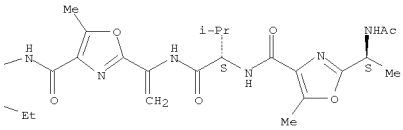
PAGE 1-A



PAGE 1-B



PAGE 1-C

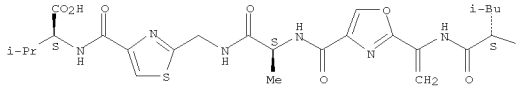


IT 884593-30-0P
RL: BPN (Biosynthetic preparation); PRP (Properties); BIOL (Biological study); PREP (Preparation)
(T5S; cloning and characterization of goadsporin biosynthetic gene cluster from Streptomyces sp. TP-A0584)

RN 884593-30-0 CAPLUS
CN L-Valine,
N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbonyl]-
L-valyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl- (9CI) (CA INDEX NAME)

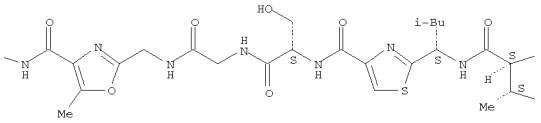
Absolute stereochemistry.

PAGE 1-A

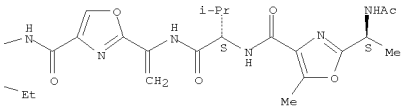


L31 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B



PAGE 1-C



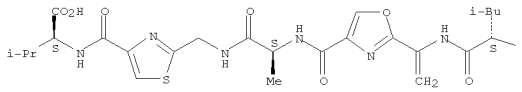
IT 403476-91-5P, Goadsporin
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(cloning and characterization of goadsporin biosynthetic gene cluster from Streptomyces sp. TP-A0584)
RN 403476-91-5 CAPLUS
CN L-Valine,
N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbonyl]-

L-valyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-

1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl- (CA INDEX NAME)

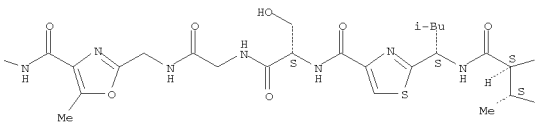
Absolute stereochemistry. Rotation (-).

PAGE 1-A

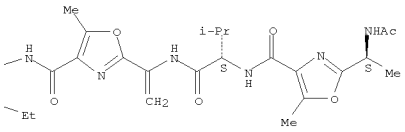


L31 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B



PAGE 1-C



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 9 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1126676 CAPLUS
DOCUMENT NUMBER: 143:405899
TITLE: Preparation of thiazoles and analogs as anaplastic lymphoma kinase modulators
INVENTOR(S): Leahy, James William; Lewis, Gary Lee; Nuss, John M.; Ridgway, Brian Hugh; Sangalang, Joan C.
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 346 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005097765	A1	20051020	WO 2005-US10969	20050331
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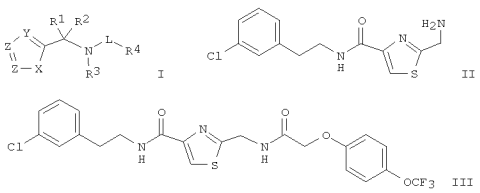
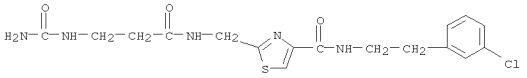
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005230847	A1	20051020	AU 2005-230847	20050331
CA 2559866	A1	20051020	CA 2005-2559866	20050331
EP 1730128	A1	20061213	EP 2005-733275	20050331
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2008502595	T	20080131	JP 2007-506579	20050331
US 20090186905	A1	20090723	US 2007-598911	20070607
PRIORITY APPLN. INFO.:			US 2004-558800P P	20040331
			WO 2005-US10969 W	20050331

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 143:405899; MARPAT 143:405899
GI

L31 ANSWER 9 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



AB Title compds. I [wherein R1, R2 = H, halo, trihalomethyl; R1 and R2 are oxo; R3, R4 = H, (un)substituted alkyl, aryl; X = O, S; Y = (un)substituted CH or N; one of Z = C(COO-alkyl), C(CONH-alkyl), while the other Z = N, (un)substituted CH; L = C(O/S), SO2 or absence; etc., pharmaceutically acceptable salts, hydrates or prodrugs thereof] as modulators of protein kinases, especially anaplastic lymphoma kinases (ALK).
For example, alkylation of 4-CF3OC6H4OH with tert-Bu bromoacetate followed by treatment with TFA and chlorination with SOCl2 gave an acyl chloride (97% yield for three steps), which underwent amidation with amine II (preparation given) to afford amide III. This compds. showed inhibition against ALK with IC50 < 50 nM in the luciferase-coupled chemiluminescent kinase assay. Therefore, I and their pharmaceutical compns. are useful for modulating protein kinase enzymic activity and for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion.
IT 1044708-62-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Preparation of thiazoles and analogs as anaplastic lymphoma kinase modulators)
RN 1044708-62-4 CAPLUS
CN 4-Thiazolecarboxamide, 2-[[[3-[(aminocarbonyl)amino]-1-oxopropyl]amino]methyl]-N-[2-(3-chlorophenyl)ethyl]- (CA INDEX NAME)



IT 867340-11-2P 867340-14-5P 867340-17-8P
867340-20-3P 867340-46-3P 867340-50-9P
867340-56-5P 867340-59-8P 867340-63-4P
867340-65-6P 867340-66-7P 867340-67-8P
867340-68-9P 867340-70-3P 867340-71-4P
867340-72-5P 867340-73-6P 867340-74-7P

(2 CITINGS)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

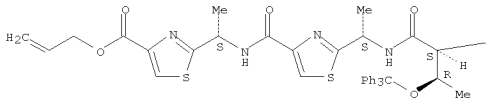
L31 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:244364 CAPLUS
DOCUMENT NUMBER: 142:482299
TITLE: Total synthesis of didmolamides A and B
AUTHOR(S): You, Shu-Li; Kelly, Jeffery W.
CORPORATE SOURCE: Department of Chemistry, Skaggs Institute for Chemical
Biology, Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Tetrahedron Letters (2005), 46(15), 2567-2570
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:482299

AB The first total synthesis of didmolamides A and B has been accomplished by
the solid phase assembly of thiazole-containing amino acids and com. available Fmoc-protected (Fmoc = 9-fluorenylmethyloxycarbonyl) amino acids. The synthesis of didmolamide B was also achieved in high yield using solution phase peptide synthesis. The thiazole-containing amino acid composing didmolamides A and B was synthesized by a MnO2 oxidation of a
thiazoline, prepared from an Ala-Cys dipeptide using bis(triphenyl)oxodiphosphonium trifluoromethanesulfonate. The final macrolactamization was accomplished efficiently by PyBOP and DMAP in solution

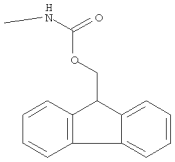
IT 851790-99-3P 851791-00-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of didmolamide B by solution coupling)
RN 851790-99-3 CAPLUS
CN 4-Thiazolecarboxylic acid, 2-[(1S)-1-[[[2-[(1S)-1-[[(2S,3R)-2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-1-oxo-3-(triphenylmethoxy)butyl]amino]ethyl]-4-thiazolyl]carbonyl]amino]ethyl]-, 2-propen-1-yl ester (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



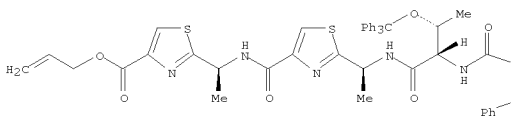
PAGE 1-B



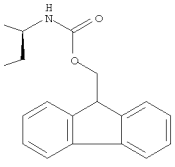
RN 851791-00-9 CAPLUS
CN L-Threoninamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-phenylalanyl-N-[(1S)-1-[4-[[[(1S)-1-[4-[(2-propenyloxy)carbonyl]-2-thiazolyl]ethyl]amino]carbonyl]-2-thiazolyl]ethyl]-O-(triphenylmethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L31 ANSWER 11 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:58514 CAPLUS
DOCUMENT NUMBER: 140:236094
TITLE: Highly efficient biomimetic total synthesis and structural verification of bistratamides E and J from Lissoclinum bistratum
AUTHOR(S): You, Shu-li; Kelly, Jeffery W.
CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Chemistry--A European Journal (2004), 10(1), 71-75
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:236094

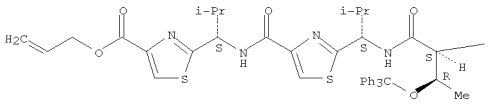
AB The interesting biol. activities of heterocycle-containing cyclic peptide-derived natural products, isolated from marine organisms over the past twenty years, have attracted the interest of many synthetic and natural products chemists. Bistratamides E-J, members of this class of natural products that were isolated very recently from Lissoclinum bistratum, exhibited cytotoxic activity against a human colon tumor (HCT-116) cell line. Here we report the first total syntheses of bistratamides E and J in overall yields of 19 and 34%, resp. The thiazole substructures have been synthesized by oxidation of their corresponding thiazoline substructures, which were obtained from cysteine containing peptides using a novel biomimetic approach wherein Val-Cys dipeptide units were converted to thiazolines by a bisphosphonium salt. The final macrocyclization was promoted efficiently using the combination of PyBOP and DMAP. This approach allows the use of readily available Fmoc-protected (Fmoc = 9-fluorenylmethyloxycarbonyl) amino acids to make complex thiazole and oxazoline-containing natural products.

IT 668489-46-1P 668489-47-2P 668489-50-7P
668489-51-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of bistratamides E and J from Lissoclinum bistratum from cysteine containing peptides via oxidation of their corresponding thiazoline substructures and macrocyclization)

RN 668489-46-1 CAPLUS
CN 4-Thiazolecarboxylic acid, 2-[(1S)-1-[[[2-[(1S)-1-[[(2S,3R)-2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-1-oxo-3-(triphenylmethoxy)butyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]amino]-2-methylpropyl]-, 2-propen-1-yl ester (CA INDEX NAME)

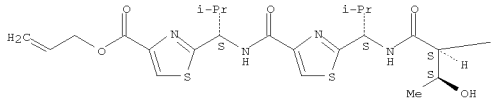
Absolute stereochemistry. Rotation (-).

PAGE 1-A

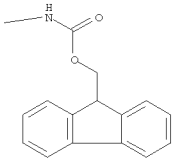


L31 ANSWER 11 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
Absolute stereochemistry. Rotation (-).

PAGE 1-A



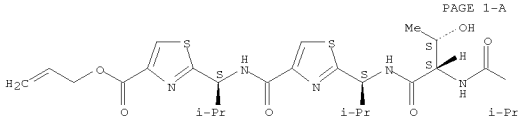
PAGE 1-B



RN 668489-51-8 CAPLUS
CN L-Allothreoninamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-valyl-N-[(1S)-2-methyl-1-[4-[[[(1S)-2-methyl-1-[4-[(2-propenyloxy)carbonyl]-2-thiazolyl]propyl]amino]carbonyl]-2-thiazolyl]propyl]- (9CI) (CA INDEX NAME)

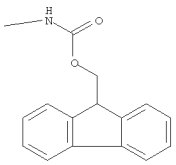
Absolute stereochemistry. Rotation (-).

PAGE 1-A



L31 ANSWER 11 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

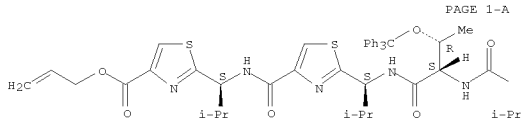
PAGE 1-B



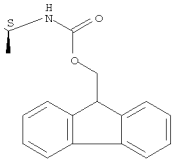
RN 668489-47-2 CAPLUS
CN L-Threoninamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-valyl-N-[(1S)-2-methyl-1-[4-[[[(1S)-2-methyl-1-[4-[(2-propenyloxy)carbonyl]-2-thiazolyl]propyl]amino]carbonyl]-2-thiazolyl]propyl]-O-(triphenylmethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



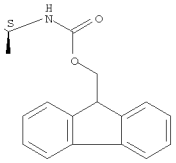
PAGE 1-B



RN 668489-50-7 CAPLUS
CN 4-Thiazolecarboxylic acid, 2-[(1S)-1-[[[2-[(1S)-1-[[(2S,3S)-2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-hydroxy-1-oxobutyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]amino]-2-methylpropyl]-, 2-propen-1-yl ester (CA INDEX NAME)

L31 ANSWER 11 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B



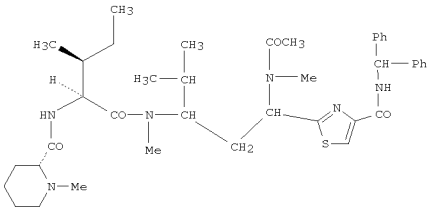
OS.CITING REF COUNT: 28 THERE ARE 28 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)
REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 12 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:41505 CAPLUS
DOCUMENT NUMBER: 140:94300
TITLE: Synthesis of tubulysin derivatives for therapeutic use
in treatment of disease
INVENTOR(S): Doemling, Alexander; Henkel, Bernd; Beck, Barbara; Illgen, Katrin; Sakamuri, Sukumar; Menon, Sanjay
PATENT ASSIGNEE(S): Morphochem Aktiengesellschaft fur Kombinatorische Chemie, Germany
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005327	A1	20040115	WO 2003-EP7419	20030709
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10230874	A1	20040122	DE 2002-10230874	20020709
DE 10252719	A1	20040527	DE 2002-10252719	20021113
AU 2003266233	A1	20040123	AU 2003-266233	20030709
EP 1523493	A1	20050420	EP 2003-762676	20030709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 20050239713	A1	20051027	US 2005-520793	20050708

PRIORITY APPLN. INFO.:			
	DE 2002-10230874	A	20020709
	DE 2002-10252719	A	20021113
	WO 2003-EP7419	W	20030709

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 140:94300
GI



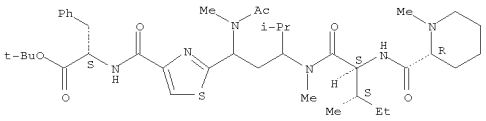
I

AB Synthesis of title compds., e.g., (I), and preparation of reactants for these syntheses, for use in the treatment of autoimmune disease or tumors via their cytostatic effect (no data) was claimed. Thus, N-methyl-β-DL-valinolyl tert-butyldiphenylsilylether (II) was prepared in three steps from methylamine, isobutyraldehyde, and malonic acid. D-N-methyl-homo-prolyl-L-isoleucine (III) was also prepared in four steps from D-N-Boc-homoproline and L-isoleucine benzyl ester. II and III were coupled, the silyl protecting group removed, and the resulting alc. subjected to Swern oxidation to give an aldehyde intermediate, which was reacted with Me 3-dimethylamino-2-isocyanoacrylate, Me amine, and thioacetic acid; the resulting 1,3-thiazole-containing compound was deesterified and reacted with various amines or amino acids to give title product I.

IT 644960-80-5P 644960-82-7P 644960-86-1P
644960-87-2P 644960-88-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tubulysin derivs. for therapeutic use in treatment of disease)

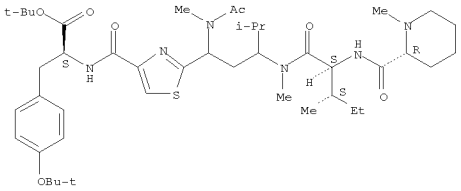
RN 644960-80-5 CAPLUS
CN L-Phenylalanine, (2R)-1-methyl-2-piperidinecarbonyl-L-isoleucyl-2-[1-(acetylmethylamino)-4-methyl-3-(methylamino)pentyl]-4-thiazolecarbonyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



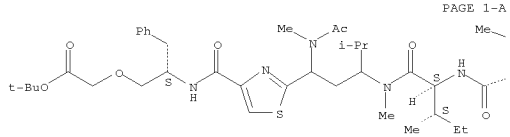
RN 644960-82-7 CAPLUS
CN L-Tyrosine, (2R)-1-methyl-2-piperidinecarbonyl-L-isoleucyl-2-[1-(acetylmethylamino)-4-methyl-3-(methylamino)pentyl]-4-thiazolecarbonyl-O-(1,1-dimethylethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



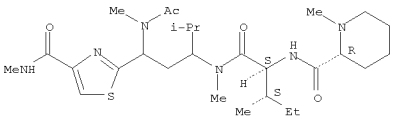
RN 644960-86-1 CAPLUS
CN Acetic acid, 2-[(2S)-2-[[[2-[1-(acetylmethylamino)-4-methyl-3-[methyl[(2S,3S)-3-methyl-2-[[[(2R)-1-methyl-2-piperidinyl]carbonyl]amino]-1-oxopentyl]amino]pentyl]-4-thiazolyl]carbonyl]amino]-3-phenylpropoxy]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



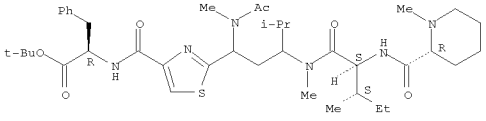
RN 644960-87-2 CAPLUS
CN 2-Piperidinecarboxamide, N-[(1S,2S)-1-[[[3-(acetylmethylamino)-3-[4-[(methylamino)carbonyl]-2-thiazolyl]-1-(1-methylethyl)propyl]methylamino]carbonyl]-2-methylbutyl]-1-methyl-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 644960-88-3 CAPLUS
CN D-Phenylalanine, (2R)-1-methyl-2-piperidinecarbonyl-L-isoleucyl-2-[1-(acetylmethylamino)-4-methyl-3-(methylamino)pentyl]-4-thiazolecarbonyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

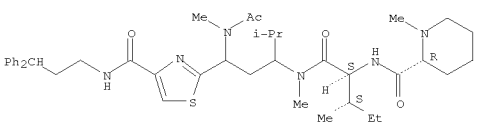
Absolute stereochemistry.



IT 644961-02-4P 644961-03-5P 644961-04-6P
644961-05-7P 644961-06-8P 644961-15-9P
644961-16-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tubulysin derivs. for therapeutic use in treatment of disease)

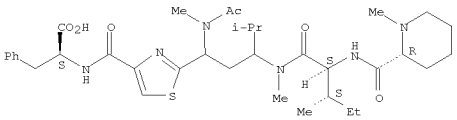
RN 644961-02-4 CAPLUS
CN 2-Piperidinecarboxamide, N-[(1S,2S)-1-[[[3-(acetylmethylamino)-3-[4-[[(3,3-diphenylpropyl)amino]carbonyl]-2-thiazolyl]-1-(1-methylethyl)propyl]methylamino]carbonyl]-2-methylbutyl]-1-methyl-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 644961-03-5 CAPLUS
CN L-Phenylalanine, (2R)-1-methyl-2-piperidinecarbonyl-L-isoleucyl-2-[1-(acetylmethylamino)-4-methyl-3-(methylamino)pentyl]-4-thiazolecarbonyl-, (9CI) (CA INDEX NAME)

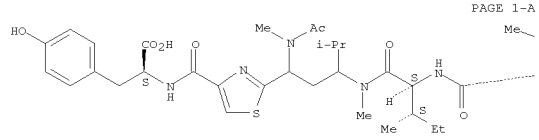
L31 ANSWER 12 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
Absolute stereochemistry.



RN 644961-04-6 CAPLUS
CN L-Tyrosine, (2R)-1-methyl-2-piperidinecarbonyl-L-isoleucyl-2-[1-(acetylmethylamino)-4-methyl-3-(methylamino)pentyl]-4-thiazolecarbonyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

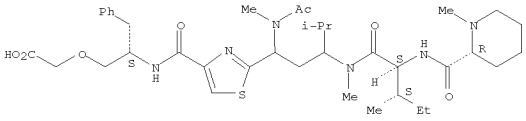
PAGE 1-A



PAGE 1-B

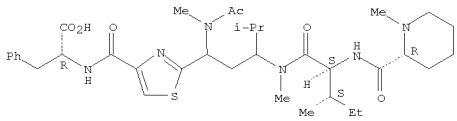
RN 644961-05-7 CAPLUS
CN Acetic acid, 2-[(2S)-2-[[[2-[1-(acetylmethylamino)-4-methyl-3-[methyl[(2S,3S)-3-methyl-2-[[[(2R)-1-methyl-2-piperidinyl]carbonyl]amino]-1-oxopentyl]amino]pentyl]-4-thiazolyl]carbonyl]amino]-3-phenylpropoxy]- (CA INDEX NAME)

Absolute stereochemistry.



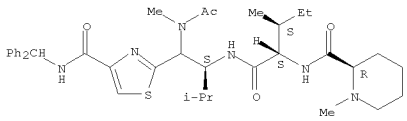
L31 ANSWER 12 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RN 644961-06-8 CAPLUS
CN D-Phenylalanine, (2R)-1-methyl-2-piperidinecarbonyl-L-isoleucyl-2-[1-(acetylmethylamino)-4-methyl-3-(methylamino)pentyl]-4-thiazolecarbonyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



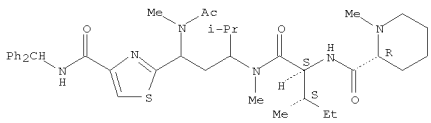
RN 644961-15-9 CAPLUS
CN 2-Piperidinecarboxamide, N-[(1S,2S)-1-[[[(1S)-1-[(acetylmethylamino)[4-[[(diphenylmethyl)amino]carbonyl]-2-thiazolyl]methyl]-2-methylpropyl]amino]carbonyl]-2-methylbutyl]-1-methyl-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 644961-16-0 CAPLUS
CN 2-Piperidinecarboxamide, N-[(1S,2S)-1-[[[3-(acetylmethylamino)-3-[4-[[(diphenylmethyl)amino]carbonyl]-2-thiazolyl]-1-(1-methylethyl)propyl]methylamino]carbonyl]-2-methylbutyl]-1-methyl-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 12 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L31 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2003:613013 CAPLUS
DOCUMENT NUMBER: 140:267690
TITLE: Determination of the absolute configuration of thiazole-containing amino acids in a peptide using the advanced Marfey's method
AUTHOR(S): Fujii, Kiyonaga; Nakano, Tomoyo; Imanishi, Susumu; Harada, Ken-ichi
CORPORATE SOURCE: Faculty of Pharmacy, Meijo University, Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (2001), 43rd, 389-394
CODEN: TYKYDS
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB A symposium report : a large number of peptides containing the modified amino acids such as thiazole (Tzl) and oxazole (Ozl) rings have been isolated from cyanobacteria and marine origins. In general, the absolute configuration of such a modified amino acid in a peptide is determined on the basis of that of the corresponding intact amino acid derived from the hydrolyzate after chemical treatments. In order to derive intact amino acids from Tzl-amino acids in a peptide, Ireland et al. proposed a method composed of acid hydrolysis combined with ozonolysis in 1983. Since then, although this method has been applied to many peptides containing Tzl-amino acids, no method has been established for the direct detection and the identification of Tzl-amino acids including the absolute configuration. The authors have established a nonempirical method using LC/MS, the advanced Marfey's method, which includes HPLC with a rational guideline, a sensitive derivatizing reagent, FDLA (1-fluoro-2,4-dinitrophenyl-5-leuciamide), and a racemization procedure using DL-FDLA, for determination of the absolute configuration of constituent amino acids and amines in a peptide. Therefore, they considered that TA-amino acids in the hydrolyzate can be directly detected and determine the absolute configuration by the "advanced Marfey's method" without ozonolysis. For the determination of the absolute configuration of Tzl-amino acids in a peptide, they applied the advanced Marfey's method to the isolated microcyclamide (I) containing two Tzl-amino acids. Tzl-amino acids could be directly detected together with a constituent amino acid in the hydrolyzate by this method, although they were racemized under ordinary hydrolysis conditions as expected. According to the proposed separation mechanism of Marfey's method, the elution order of Tzl-amino acids can be basically determine in the same way as amino acids. In order to identify each original peak of Tzl-amino acids, the flash hydrolysis (6M HCl, 110°C, 1 h) was introduced for the control of the racemization during the acid hydrolysis. Consequently, the absolute configuration of I containing Tzl-amino acids was clearly determined Addnl., this method with the flash hydrolysis was successfully applied to

L31 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

the detn. of the abs. configuration of constituent amino acids in two naturally occurring peptides, waiakeamide and goadsporin, possessing TA-amino acids. The methodol. using LC/MS combined with flash hydrolysis is being further extended for the structural detn. of various naturally occurring peptides possessing the modified amino acids and D-amino acids.

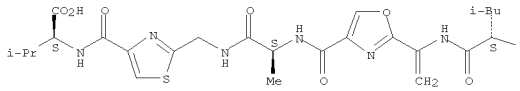
IT 403476-91-5, Goadsporin
RL: PRP (Properties)
(determination of the absolute configuration of thiazole-containing amino
acids in a peptide using the advanced Marfey's method)

RN 403476-91-5 CAPLUS

CN L-Valine, N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbonyl]-
L-valyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-
1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



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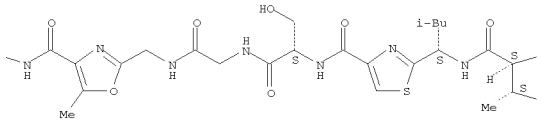
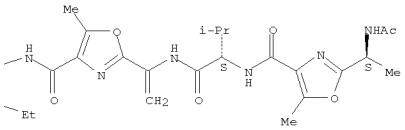


L31 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-C



L31 ANSWER 14 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:521317 CAPLUS
DOCUMENT NUMBER: 139:239657
TITLE: Structure-based design of agents targeting the bacterial ribosome
AUTHOR(S): Bower, Justin; Drysdale, Martin; Hebdon, Richard; Jordan, Allan; Lentzen, Georg; Matassova, Natalia; Murchie, Alastair; Powles, Jenifer; Roughley, Stephen
CORPORATE SOURCE: Department of Medicinal Chemistry, RiboTargets Ltd., Abington, Cambridge, CB1 6GB, UK
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(15), 2455-2458
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:239657

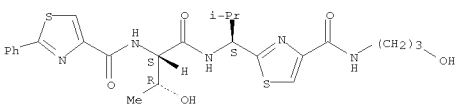
AB Rational structure-based drug design has been applied to the antibiotic thiostrepton, to overcome some of its' limitations. The identification of
a proposed binding fragment allowed construction of a number of key fragments, which were derivatized to generate a library of potential antibiotics. These were then evaluated to determine their ability to bind to
the L11 binding domain of the prokaryotic ribosome and inhibit bacterial protein translation.

IT 666235-45-6P 666235-50-3P 666235-51-4P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(structure-based design of agents targeting the bacterial ribosome)

RN 666235-45-6 CAPLUS

CN 4-Thiazolecarboxamide, N-[(1S,2R)-2-hydroxy-1-[[[(1S)-1-[4-[[(3-hydroxypropyl)amino]carbonyl]-2-thiazolyl]-2-methylpropyl]amino]carbonyl]propyl]-2-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

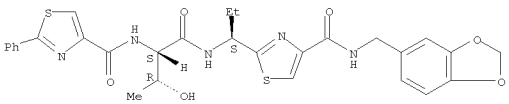


RN 666235-50-3 CAPLUS

CN 4-Thiazolecarboxamide, N-[(1S,2R)-1-[[[(1S)-1-[4-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-2-thiazolyl]propyl]amino]carbonyl]-2-hydroxypropyl]-2-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

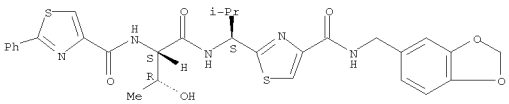
L31 ANSWER 14 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 666235-51-4 CAPLUS

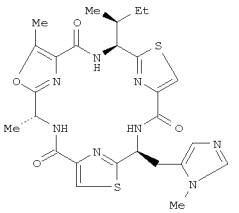
CN 4-Thiazolecarboxamide, N-[(1S,2R)-1-[[[(1S)-1-[4-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-2-thiazolyl]-2-methylpropyl]amino]carbonyl]-2-hydroxypropyl]-2-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 15 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2002:641298 CAPLUS
DOCUMENT NUMBER: 138:39527
TITLE: Simultaneous detection and determination of the absolute configuration of thiazole -containing amino acids in a peptide
AUTHOR(S): Fujii, Kiyonaga; Yahashi, Yukie; Nakano, Tomoyo; Imanishi, Susumu; Baldia, Susana F.; Harada, Ken-ichi
CORPORATE SOURCE: Faculty of Pharmacy, Meijo University, Tempaku, Nagoya, 468-8503, Japan
SOURCE: Tetrahedron (2002), 58(34), 6873-6879
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

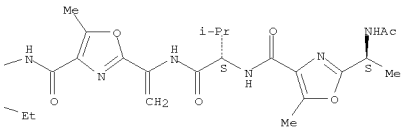


I

AB For the simultaneous detection and determination of the absolute configuration of a thiazole-containing (Tzl-) amino acid in a peptide, we have developed a reliable method using the 'advanced Marfey's method', which includes HPLC with a rational guideline, a sensitive derivatizing reagent, 1-fluoro-2,4-dinitrophenyl-5-L-leucinamide (L-FDLA), and a racemization procedure using DL-FDLA for determination of the absolute configuration of constituent amino acids in a peptide. Tzl-amino acids could be directly detected in the hydrolyzate by this method, although they were racemized under ordinary hydrolysis conditions. In order to depress the racemization, the flash hydrolysis was introduced. As a result, the flash hydrolysis for 1 h was sufficient to detect each constituent amino acid, and it was possible to identify the original peak. Consequently, the absolute configuration of microcyclamide I possessing Tzl-amino acids was determined by the advanced Marfey's method combined with flash hydrolysis. At 13.7 and 26.6 μg/mL (IC50) I showed a cytotoxicity against the lymphocytic mouse leukemia and showed an anticyanobacterial activity against Anabaena sp. Addnl., this method was successfully applied to the simultaneous detection and determination of the absolute configuration of two other naturally occurring

L31 ANSWER 15 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-C



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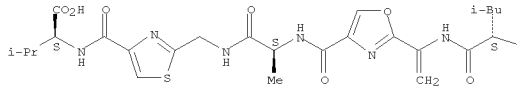
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 15 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
peptides, waiakeamide and goadsporin. The established method with the flash hydrolysis had an addnl. advantage in that labile amino acids, such as tryptophan and methionine sulfoxide, during acid hydrolysis can be detected in the intact form.
IT 403476-91-5, Goadsporin
RL: ANT (Analyte); PRP (Properties); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent)
(detection and determination of absolute configuration of thiazole -containing amino acids in naturally occurring peptides waiakeamide and goadsporin)
RN 403476-91-5 CAPLUS
CN L-Valine, N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbonyl]-L-valyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



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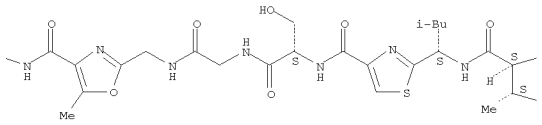
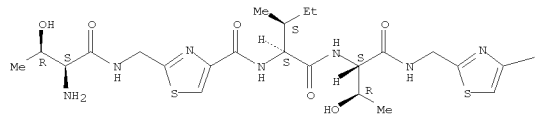


L31 ANSWER 16 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2002:290336 CAPLUS
DOCUMENT NUMBER: 137:87443
TITLE: Synthesis and structural properties of patellamide A derivatives and their copper(II) compounds
AUTHOR(S): Bernhardt, Paul V.; Comba, Peter; Fairlie, David P.; Gahan, Lawrence R.; Hanson, Graeme R.; Lotzbeyer, Lutz
CORPORATE SOURCE: Department of Chemistry, The University of Queensland, Brisbane, 4072, Australia
SOURCE: Chemistry--A European Journal (2002), 8(7), 1527-1536
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:87443
AB The synthesis, characterization and Cu(II) coordination chemical of three new cyclic peptide ligands, PatJ1 (cyclo-(Ile-Thr-(Gly)Thz-Ile-Thr-(Gly)Thz)), PatJ2 (cyclo-(Ile-Thr-(Gly)Thz-(D)-Ile-Thr-(Gly)Thz)), and PatL (cyclo-(Ile-Ser-(Gly)Thz-Ile-Ser-(Gly)Thz)) are reported. All of these cyclic peptides and PatN (cyclo-(Ile-Ser-(Gly)Thz-Ile-Thr-(Gly)Thz)) are derivs. of patellamide A and have a [24]azacrown-8 macrocyclic structure. All four synthetic cyclic peptides have two thiazole rings but, in contrast to patellamide A, no oxazoline rings. The mol. structure of PatJ1, determined by x-ray crystallog., has a saddle conformation with two close-to-coparallel thiazole rings, very similar to the geometry of patellamide D. The two coordination sites of PatJ1 with thiazole-N and amide-N donors are each well preorganized for transition metal ion binding. The coordination of Cu(II) was monitored by UV/visible spectroscopy, and this reveals various (meta)stable mono- and dinuclear Cu(II) complexes whose stoichiometry was confirmed by mass spectra. Two types of dinuclear Cu(II) complexes, [Cu2(H4L)(OH2)n]2+ (n = 6, 8) and [Cu2(H2L)(OH2)n] (n = 4, 6; L = PatN, PatL, PatJ1, PatJ2) were identified and analyzed structurally by EPR spectroscopy and a combination of spectra simulations and mol. mechanics calcns. (MM-EPR). The four structures are similar to each other and have a saddle conformation, i.e., derived from the crystal structure of PatJ1 by a twist of the two thiazole rings. The small but significant structural differences were characterized by the EPR simulations.
IT 439858-32-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of cyclic peptide analog of patellamide A)
RN 439858-32-9 CAPLUS
CN L-Isoleucine, L-threonyl-2-(aminomethyl)-4-thiazolecarbonyl-L-isoleucyl-L-threonyl-2-(aminomethyl)-4-thiazolecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 16 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A



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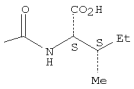

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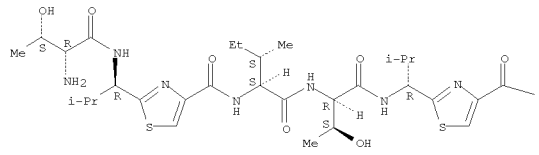
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 17 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
thiazolecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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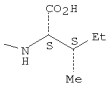

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REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 17 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2002:289497 CAPLUS
DOCUMENT NUMBER: 137:20592
TITLE: Cyclic octapeptides containing thiazole. Effect of stereochemistry and degree of flexibility on calcium binding properties
AUTHOR(S): Cusack, Rodney M.; Grondahl, Lisbeth; Fairlie, David P.; Gahan, Lawrence R.; Hanson, Graeme R.
CORPORATE SOURCE: Chemistry Department, The University of Queensland, Brisbane, 4072, Australia
SOURCE: Journal of the Chemical Society, Perkin Transactions 2
(2002), (3), 556-563
CODEN: JCSPGI; ISSN: 1472-779X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:20592

AB Solution conformation and calcium binding properties have been investigated for the two cyclic octapeptides cyclo-(-D-Thr-D-Val(Thz)-Ile-)2 (I) and cyclo(-Thr-Gly(Thz)-Ile-Ser-Gly(Thz)-Ile-) (II) and the results are compared to those for the cyclic octapeptides previously studied; ascidiacyclamide (III), patellamide D (IV), cyclo(-Thr-D-Val(Thz)-Ile-)2 (V), and cyclo(-Thr-D-Val-αAbu-Ile-)2 (VI). Both I and II contain two heterocyclic thiazole ring constraints but the latter has a larger degree of flexibility as a consequence of the glycine residues within the cyclic framework. The solution conformation of I and II was determined from 1H NMR spectra and found to be a "twisted figure of eight" similar to that for IV. Complexation studies using 1H NMR and CD spectroscopy yielded 1: 1 calcium-peptide binding consts. (logK) for the two peptides (2.3 (I) and 5.7 (II)). For II the magnitude of the binding constant was verified by a competition titration using CD. The different calcium-binding affinities of V (logK = 4.0) and I is attributed to the stereochem. of the threonine residue. The magnitude of the binding constant for II compared to V and I (all peptides containing two thiazole ring constrains) demonstrates that the increase in flexibility of the cyclic peptide has a dramatic effect on the Ca2+ binding ability. The affinity for Ca2+ thus decreases in the order (VI .apprx. II > V > IV .apprx. III > I). The number of carbonyl donors available on each peptide has only a limited effect on calcium binding. The most important factor is the flexibility, which allows for a conformation of the peptide capable of binding calcium efficiently.

IT 434335-13-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, conformation, and calcium-binding properties of two synthetic cyclooctapeptides compared to sea squirt cyclooctapeptides)

RN 434335-13-4 CAPLUS
CN L-Isoleucine, D-threonyl-2-[(1R)-1-amino-2-methylpropyl]-4-thiazolecarbonyl-L-isoleucyl-D-threonyl-2-[(1R)-1-amino-2-methylpropyl]-4-

L31 ANSWER 18 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2002:11959 CAPLUS
DOCUMENT NUMBER: 136:263447
TITLE: Goadsporin, a chemical substance which promotes secondary metabolism and morphogenesis in streptomycetes. II. Structure determination
AUTHOR(S): Igarashi, Yasuhiro; Kan, Yukiko; Fujii, Kiyonaga; Fujita, Tsuyoshi; Harada, Ken-Ichi; Naoki, Hideo; Tabata, Hirokazu; Onaka, Hiroyasu; Furumai, Tamotsu
CORPORATE SOURCE: Biotechnology Research Center, Toyama Prefectural University, Toyama, 939-0398, Japan
SOURCE: Journal of Antibiotics (2001), 54(12), 1045-1053
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English

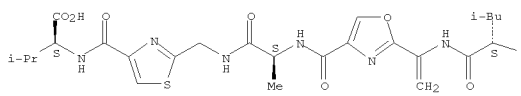
AB The structure of goadsporin was determined by using spectroscopic techniques. NMR anal. revealed that goadsporin consists of 19 amino acids, two of which are dehydroalanines (Deala), and six of which are cyclized to oxazoles (Oxz) and thiazoles (Thz) by dehydrative cyclization and dehydrogenation from serine, threonine and cysteine. NMR anal. established seven partial structures, and their sequence was determined by CID-MS/MS. Neg. mode FAB-MS/MS gave product ions arising from charge-remote fragmentation that allowed determination of the sequence of the amino acid components as AcNH-Ala-MeOxz-Val-Deala-MeOxz-Ile-Leu-Thz-Ser-Gly-Gly-MeOxz-Leu-Deala-Oxz-Ala-Gly-Thz-Val-OH. The chiral amino acids were determined by the advanced Marfey's method to have L-configurations.

IT 403476-91-5, Goadsporin
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(structure determination of the antibiotic goadsporin using NMR and CID-MS/MS)

RN 403476-91-5 CAPLUS
CN L-Valine, N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbonyl]-L-valyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



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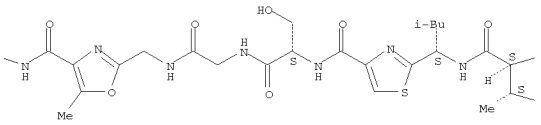

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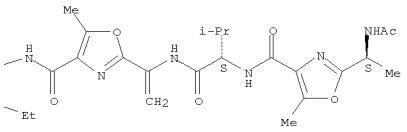


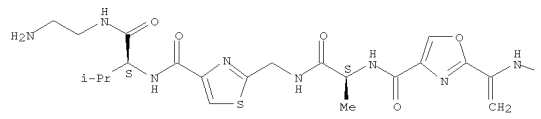
IT 405202-94-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(structure determination of the antibiotic goadsporin using NMR and CID-MS/MS)
RN 405202-94-0 CAPLUS
CN L-Valinamide, N-[[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-

oxazolyl]carbonyl]-L-valyl-2-(1-aminoethenyl)-5-methyl-4-oxazolecarbonyl-L-

isoleucyl-2-[(1S)-1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminoethenyl)-4-oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl-N-(2-aminoethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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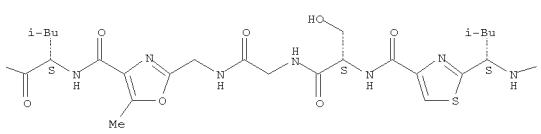

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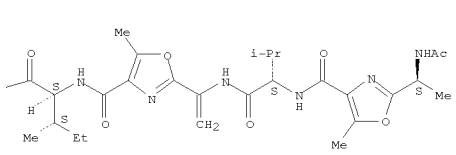

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REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2001:526422 CAPLUS
DOCUMENT NUMBER: 135:269150
TITLE: In vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bisheterocyclic sites
AUTHOR(S): Zamble, Deborah B.; Miller, Deborah A.; Heddle, Jonathan G.; Maxwell, Anthony; Walsh, Christopher T.; Hollfelder, Florian
CORPORATE SOURCE: Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2001), 98(14), 7712-7717
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Microcin B17 (MccB17) is a 3.1-kDa Escherichia coli antibiotic that contains thiazole and oxazole heterocycles in a peptide backbone. MccB17 inhibits its cellular target, DNA gyrase, by trapping the enzyme in a complex that is covalently bound to double-strand cleaved DNA, in a manner similar to the well-known quinolone drugs. The identification of gyrase as the target of MccB17 provides an opportunity to analyze the relationship between the structure of this unusual antibiotic and its activity. In this report, steady-state parameters are used to describe the induction of the cleavable complex by MccB17 analogs containing modified bis-heterocyclic sites. The relative potency of these analogs corresponds to the capacity of the compds. to prevent growth of sensitive cells. In contrast to previously reported expts., inhibition of DNA gyrase supercoiling activity by wild-type MccB17 also was observed These results suggest that DNA gyrase is the main intracellular target of MccB17. This study probes the structure-function relationship of a new class of gyrase inhibitors and demonstrates that these techniques could be used to analyze compds. in the search for clin. useful antibiotics that block DNA gyrase.
IT 84286-90-8, microcin B17 84286-90-8D, microcin B17, analogs 234125-07-6 234125-08-7
234125-11-2 234125-15-6 234125-18-9
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(in vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bis-heterocyclic sites)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-

(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-

(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 234125-07-6 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonyl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-

asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 234125-08-7 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2'-(aminomethyl)[2,4'-bithiazole]-4-carbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-

(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 234125-11-2 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2'-

(aminomethyl)[2,4'-bithiazole]-4-carbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 234125-15-6 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-(aminomethyl)-4-thiazolecarbonylglycylglycylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

L31 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 234125-18-9 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginylglycylglycylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 20 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2000:900812 CAPLUS
DOCUMENT NUMBER: 134:70356
TITLE: Avirulent brucella with mutated BacA gene and its uses as vaccines
INVENTOR(S): Levier, Kristin; Walker, Graham C.; Roop, Roy M., II; Phillips, Robert W.; Robertson, Gregory T.
PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000077213	A2	20001221	WO 2000-US15949	20000609
WO 2000077213	A3	20010705		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-138751P P 19990611

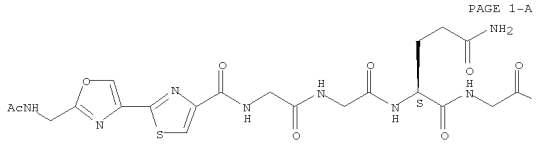
AB The present invention discloses a novel approach to attenuating bacteria and their us as live vaccines. In particular, there is disclosed a method of attenuating bacteria Brucella (B.) abortus by mutating bacA gene, which encodes a membrane protein. The amino acid alignment of BacA from B. abortus, the BacA homolog of R. meliloti, and SbmA from E. coli are provided. The invention also relates to constructing BacA gene expression vector and mutagenesis of BacA gene for preparation avirulent Brucella strain used as vaccines. The invention also discloses methods of deliver compds. into cells by BacA mediated transport and drug screening methods by identifying BacA ligands.
IT 84286-90-8, Microcin B17
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(antibiotics; avirulent brucella with mutated BacA gene and uses as vaccines)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

L31 ANSWER 20 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L31 ANSWER 21 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2000:894828 CAPLUS
DOCUMENT NUMBER: 134:208109
TITLE: Design, synthesis, and antibacterial activity of a peptidomimetic library
AUTHOR(S): Hu, Bi-Huang; Martin, Lenore M.
CORPORATE SOURCE: Department of Biomedical Sciences, College of Pharmacy, University of Rhode Island, Kingston, RI, 02881-0809, USA
SOURCE: Peptides for the New Millennium, Proceedings of the American Peptide Symposium, 16th, Minneapolis, MN, United States, June 26-July 1, 1999 (2000), Meeting Date 1999, 746-747. Editor(s): Fields, Gregg B.; Tam, James P.; Barany, George. Kluwer Academic Publishers: Dordrecht, Neth.
CODEN: 69ATHX
DOCUMENT TYPE: Conference
LANGUAGE: English
AB A symposium report. Building blocks 2-(Fmoc-aminomethyl)thiazole -4-carboxylic acid (A), 2-(Fmoc-aminomethyl)oxazole-4-carboxylic acid (B), and 2-[2'-(Fmoc-aminomethyl)oxazole-4'-yl]thiazole-4-carboxylic acid (C) (Fmoc = fluorenylmethoxycarbonyl) were prepared and applied to the synthesis of a library of peptidomimetics. Ac-C-G-B-NH(CH2)3NH2, Ac-C-G-C-NH(CH2)3NH2, and Ac-C-GGQGG-A-NH(CH2)3NH2 were assayed for antibacterial activity.
IT 297165-35-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(design, synthesis, and antibacterial activity of peptidomimetic library)
RN 297165-35-6 CAPLUS
CN Glycinamide, N-[[2-[2-[(acetylamino)methyl]-4-oxazolyl]-4-thiazolyl]carbonyl]glycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonyl- (9CI) (CA INDEX NAME)

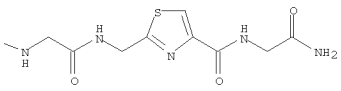
Absolute stereochemistry.

PAGE 1-A



L31 ANSWER 21 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L31 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2000:688229 CAPLUS
DOCUMENT NUMBER: 133:267157
TITLE: Preparation of peptidomimetic oxazole and thiazole combinatorial libraries
INVENTOR(S): Martin, Lenore M.; Hu, Bi-Huang
PATENT ASSIGNEE(S): Board of Governors for Higher Education, State of Rhode Island and Providence, USA
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000056724	A1	20000928	WO 2000-US7564	20000322
W: CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2368026	A1	20000928	CA 2000-2368026	20000322
EP 1169311	A1	20020109	EP 2000-919521	20000322
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002540106	T	20021126	JP 2000-606585	20000322
US 20060161007	A1	20060720	US 2005-266046	20051103
US 20100113305	A1	20100506	US 2010-684383	20100108
PRIORITY APPLN. INFO.:			US 1999-125501P	P 19990322
			WO 2000-US7564	W 20000322
			US 2002-936972	B1 20020123
			US 2005-266046	A1 20051103

OTHER SOURCE(S): MARPAT 133:267157

AB This invention utilizes synthetic heterocyclic amino acids containing thiazole and/or oxazole as building blocks in a solid phase combinatorial synthesis to yield natural and unnatural antibiotic compds. Thus, 2-(Fmoc-aminomethyl)thiazole-4-carboxylic acid (A), 2-(Fmoc-aminomethyl)oxazole-4-carboxylic acid (B), and 2-[(2'-Fmoc-aminomethyl)oxazole-4'-yl]thiazole-4-carboxylic acid (C) (Fmoc = fluorenylmethoxycarbonyl) were prepared Thus, a library of peptides Ac-X-G-X'-NH(CH2)3NH2 (X, X' are the amino acids A, B, or C and G is glycine) was prepared and individual compds. assayed for antibacterial activity.

IT 297165-35-6P 297165-43-6P 297165-44-7P
297165-45-8P 297165-46-9P 297165-49-2P
297165-51-6P 297165-53-8P 297165-55-0P
297165-57-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidomimetic oxazole and thiazole combinatorial libraries as antibiotics)

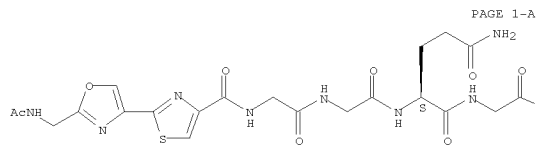
RN 297165-35-6 CAPLUS
CN Glycinamide, N-[[2-[2-[(acetylamino)methyl]-4-oxazolyl]-4-

L31 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

thiazolyl]carbonyl]glycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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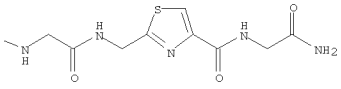
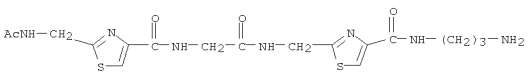
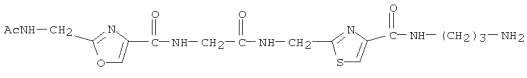


RN 297165-43-6 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(acetylamino)methyl]-N-[2-[[[4-[[(3-aminopropyl)amino]carbonyl]-2-thiazolyl]methyl]amino]-2-oxoethyl]- (CA INDEX NAME)



RN 297165-44-7 CAPLUS
CN 4-Oxazolecarboxamide, 2-[(acetylamino)methyl]-N-[2-[[[4-[[(3-aminopropyl)amino]carbonyl]-2-thiazolyl]methyl]amino]-2-oxoethyl]- (CA INDEX NAME)



RN 297165-45-8 CAPLUS
CN 4-Thiazolecarboxamide, 2-[2-[(acetylamino)methyl]-4-oxazolyl]-N-[2-[[[4-

L31 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

[[(3-aminopropyl)amino]carbonyl]-2-thiazolyl]methyl]amino]-2-oxoethyl]- (CA INDEX NAME)

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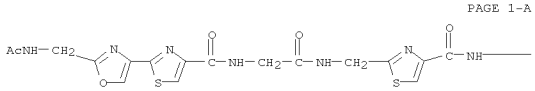
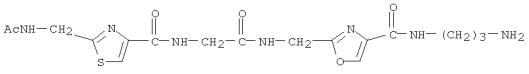


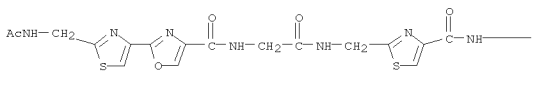
PAGE 1-B

RN 297165-46-9 CAPLUS
CN 4-Oxazolecarboxamide, 2-[[[2-[[[2-[(acetylamino)methyl]-4-thiazolyl]carbonyl]amino]acetyl]amino]methyl]-N-(3-aminopropyl)- (CA INDEX NAME)



RN 297165-49-2 CAPLUS
CN 4-Oxazolecarboxamide, 2-[2-[(acetylamino)methyl]-4-thiazolyl]-N-[2-[[[4-[[(3-aminopropyl)amino]carbonyl]-2-thiazolyl]methyl]amino]-2-oxoethyl]- (CA INDEX NAME)

PAGE 1-A

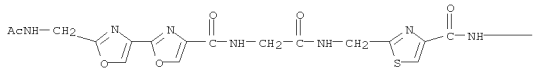


PAGE 1-B

RN 297165-51-6 CAPLUS
CN [2,4'-Bioxazole]-4-carboxamide, 2'-[(acetylamino)methyl]-N-[2-[[[4-[[(3-aminopropyl)amino]carbonyl]-2-thiazolyl]methyl]amino]-2-oxoethyl]- (CA INDEX NAME)

L31 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

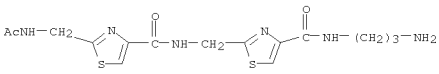
PAGE 1-A



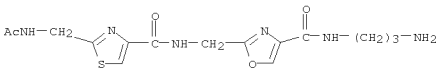
PAGE 1-B

— $(CH_2)_3$ — NH_2

RN 297165-53-8 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(acetylamino)methyl]-N-[[4-[[(3-aminopropyl)amino]carbonyl]-2-thiazolyl]methyl]- (CA INDEX NAME)

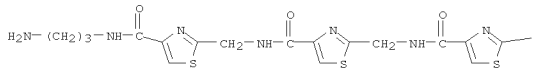


RN 297165-55-0 CAPLUS
CN 4-Oxazolecarboxamide, 2-[[[[2-[(acetylamino)methyl]-4-thiazolyl]carbonyl]amino]methyl]-N-(3-aminopropyl)- (CA INDEX NAME)



RN 297165-57-2 CAPLUS
CN 4-Thiazolecarboxamide, 2-[[[[2-[(acetylamino)methyl]-4-thiazolyl]carbonyl]amino]methyl]-N-[[4-[[(3-aminopropyl)amino]carbonyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



L31 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

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OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 23 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2000:411835 CAPLUS
DOCUMENT NUMBER: 133:132166
TITLE: Lantibiotics and microcins. Polypeptides with unusual chemical diversity
AUTHOR(S): Jack, Ralph W.; Jung, Gunther
CORPORATE SOURCE: Institut fur Organische Chemie, der Universitat Tubingen, Tubingen, 72076, Germany
SOURCE: Current Opinion in Chemical Biology (2000), 4(3), 310-317
CODEN: COCBF4; ISSN: 1367-5931
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 58 refs. is given. Bacterial-derived antimicrobial polypeptides enjoy a large degree of structural and chemical diversity.
2
Well-studied examples of such polypeptides are the lanthionine-containing lantibiotics produced by a variety of gram-pos. bacteria, and their gram-neg. counterparts, the microcins. Both groups are produced as gene-encoded precursor peptides and undergo post-translational modification to generate the active moieties. Structure elucidation of novel lantibiotics and microcins has recently uncovered further novel structural and chemical features and, combined with the generation of analog
peptides by genetic manipulation, new insights into structure-function relationships were gained. Furthermore, study of the mode of action of the lantibiotics nisin and mersacidin has revealed their use of a "docking
mol." in the target cell to facilitate their biol. activities. Meanwhile,
in vitro studies with microcin B17 have helped to uncover the mol. mechanisms by which post-translational modification results in the formation of heterocyclic oxazole and thiazole rings. Both groups of polypeptides represent new lead structures for future development of antimicrobial agents, while the identification of the "docking mols." represents a step forward in the search for novel targets for future antibiosis.
IT 84286-90-8, Microcin B17
RL: BAC (Biological activity or effector, except adverse); BPR (Biological
process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(structure, biosynthesis, and activity of microcins)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-
(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 91 THERE ARE 91 CAPLUS RECORDS THAT CITE THIS RECORD (91 CITINGS)
REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS

L31 ANSWER 23 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 24 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2000:286495 CAPLUS
DOCUMENT NUMBER: 133:89785
TITLE: Computational analysis of the first biheterocyclization site of the antibiotic microcin B17
AUTHOR(S): Donnelly, Maria A.; Zimmer, Marc
CORPORATE SOURCE: Department of Chemistry, Connecticut College, New London, CT, 06320, USA
SOURCE: Journal of Biomolecular Structure & Dynamics (2000), 17(5), 779-785
CODEN: JBSDD6; ISSN: 0739-1102
PUBLISHER: Adenine Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Microcin B17 (MccB17) undergoes an enzyme catalyzed post-translational modification to form four oxazole and four thiazole rings. Four of these rings form 4,2 - connected biheterocyclic functionalities. In this study, the hexapeptide sequence surrounding the first biheterocyclization site of microcin B17 was examined using computational calcns. and database anal. to see if it was preorganized for cyclization in a manner similar to that found in the autocatalytic post-translational cyclization of Green Fluorescent Protein (GFP). Attention was focused on the intermol. distances between the sulfur and oxygen atoms of the cysteine and serine residues and the carbonyl carbons which they attack in the ring formation. Conformational searches located some low energy conformations that contained relatively short oxygen to carbonyl carbon distances, which indicated that the oxazole forming fragment in microcin B17 is preorganized for cyclization. However, the lack of any clear patterns for the sulfur to carbon distances show that the side-chain of cysteine does not adopt any low energy conformations that are geometrically preorganized for cyclization. The MccB17 synthetase enzyme complex which catalyzes the cyclization process therefore has both steric and electronic functions. The data obtained in this investigation is in agreement with empirical data which shows that biheterocyclization will only occur if the thiazole forms before the oxazole.
IT 84286-90-8P, Microcin B 17
RL: BPN (Biosynthetic preparation); PRP (Properties); BIOL (Biological study); PREP (Preparation)
(computational anal. of the first biheterocyclization site of the antibiotic microcin B17)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 25 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1999:745504 CAPLUS
DOCUMENT NUMBER: 132:148433
TITLE: Expressed protein ligation to probe regiospecificity of heterocyclization in the peptide antibiotic microcin B17
AUTHOR(S): Roy, Ranabir Sinha; Allen, Owen; Walsh, Christopher T.
CORPORATE SOURCE: Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Chemistry & Biology (1999), 6(11), 789-799
CODEN: CBOLE2; ISSN: 1074-5521
PUBLISHER: Current Biology Publications
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The Escherichia coli peptide antibiotic microcin B17 (MccB17) contains thiazole and oxazole heterocycles derived from a distributive yet directional cyclization of cysteines and serines in the McbA precursor catalyzed by MccB17 synthetase. Whether the formation of upstream rings potentiates downstream heterocyclization has not been previously determined McbA fragments (46-61 residues) containing glycine substitutions or homocysteine at select upstream cysteine or serine sites were assembled using expressed protein ligation (EPL). Most of these substrates were only partially cyclized by MccB17 synthetase, in contrast to the efficient processing of wild-type McbA1-61. Homocysteine was not processed to the six-membered heterocycle. The formation of upstream rings in McbA potentiates the cyclization of carboxy-terminal cysteines and serines, probably by selecting against unfavorable substrate conformations. EPL allows structure-function anal. including unnatural amino acid placements to probe the regiospecificity and chemoselectivity of post-translational heterocyclization during antibiotic maturation.
IT 84286-90-8, Microcin B17
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(expressed protein ligation to probe regiospecificity of heterocyclization in the peptide antibiotic microcin b)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 26 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1999:709804 CAPLUS
DOCUMENT NUMBER: 132:50247
TITLE: Thiazole and oxazole building blocks for combinatorial synthesis
AUTHOR(S): Martin, Lenore M.; Hu, Bi-Huang
CORPORATE SOURCE: The Department of Biomedical Sciences, The University of Rhode Island, Kingston, RI, 02881-0809, USA
SOURCE: Tetrahedron Letters (1999), 40(45), 7951-7953
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:50247
AB Three thiazole and oxazole containing amino acids were synthesized in good yields by condensation-cyclization. The active functional groups used, a C-terminal imino ester or a C-terminal aldehyde, reacted with both the amino groups and side chains of either serine or cysteine within 5 min at room temperature to form oxazolines or diasteriomeric mixts. of thiazolidines, resp. The intermediate heterocyclic rings were then dehydrogenated to form the more stable, fully aromatic, rings. Ready availability of N-protected thiazole and oxazole-containing building blocks facilitates the solid-phase synthesis of natural products such as microcin B17 and other peptide-derived natural products that contain 2,4-linked thiazole and oxazole rings.
IT 84286-90-8P, Microcin B17
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of oxazole and thiazole-containing amino acids via cyclocondensation and dehydrogenation for combinatorial synthesis of peptide-derived. natural products)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 27 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1999:699662 CAPLUS
DOCUMENT NUMBER: 132:60873
TITLE: Posttranslational Heterocyclization of Cysteine and Serine Residues in the Antibiotic Microcin B17: Distributivity and Directionality
AUTHOR(S): Kelleher, Neil L.; Hendrickson, Christopher L.; Walsh, Christopher T.
CORPORATE SOURCE: Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Biochemistry (1999), 38(47), 15623-15630
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB To produce the antibiotic Microcin B17, four Cys and four Ser residues are converted into four thiazoles and four oxazoles by the three subunit Microcin B17 synthetase. High-resolution mass spectrometry (MS) was used to monitor the kinetics of posttranslational heterocyclic ring formation (-20 Da per ring) and demonstrated the accumulation of all intermediates, from one to seven rings, indicating distributive processing. All of the intermediates could be converted by the enzyme to the eight ring product. Enzymic chemoselectivity (Cys vs Ser cyclization rates) was assessed using iodoacetamido-salicylate to alkylate unreacted cysteines (+193 Da) in the 8 kDa biosynthetic intermediates; three of the first four rings formed were thiazoles, and by the five ring stage, all four of the cysteines had been heterocyclized while three of the original four serines remained uncyclized. Finally, tandem MS using a 9.4 T Fourier transform instrument with electrospray ionization was used to elaborate the major processing pathway: the first two rings formed are at the most amino proximal sites (Cys41 then Ser40) followed by the remaining three cysteines at positions 48, 51, and 55. The cyclization of serines at positions 56, 62, and 65 then follows, with Ser62 and Ser65 the last to heterocyclize and the first of these at a slower rate. Thus, despite free dissociation of intermediates after each of seven ring-forming catalytic cycles, there is an overall directionality of ring formation from N-terminal to C-terminal sites. This remarkable regioselectivity is determined more by the substrate than the enzyme, due to a combination of (1) initial high-affinity binding of the posttranslational catalyst to the N-terminal propeptide of substrate 88mer, and (2) a chemoselectivity for thiazole over oxazole formation. This mechanism is consistent with antibiotic biosynthesis in vivo, yielding microcin with six, seven, and eight rings, all with bioactivity.
IT 84286-90-8, Microcin B 17
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(posttranslational heterocyclization of cysteine and serine residues in the antibiotic microcin B17 in relation to distributivity and directionality)
RN 84286-90-8 CAPLUS

L31 ANSWER 27 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 35 THERE ARE 35 CAPLUS RECORDS THAT CITE THIS RECORD (35 CITINGS)
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 28 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1999:648054 CAPLUS
DOCUMENT NUMBER: 132:36007
TITLE: Synthesis of thiazole, imidazole and oxazole containing amino acids for peptide backbone modification
AUTHOR(S): Stankova, Ivanka G.; Videnov, Georgi I.; Golovinsky, Evgeny V.; Jung, Guenther
CORPORATE SOURCE: Department of Chemistry, Southwest University "N. Rilski", Blagoevgrad, 2700, Bulg.
SOURCE: Journal of Peptide Science (1999), 5(9), 392-398
CODEN: JPSIEI; ISSN: 1075-2617
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Novel 5-membered heterocyclic ring-containing amino acid building blocks are synthesized. These can be incorporated into analogs of peptide antibiotics such as microcin B17, which is a potent DNA-gyrase inhibitor that exhibits eight thiazole and oxazole moieties. In particular, the syntheses of imidazole and bisoxazole amino acids as novel peptidomimetics are reported, this includes a new procedure for the oxidative conversion of the intermediates oxazoline, imidazoline as well as oxazole-oxazoline into the corresponding heteroarom. compds. A mixture of DBU/CCl4/MeCN and pyridine proved to be a very effective and mild agent for this oxidation step.
IT 84286-90-8P, Microcin B17
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of thiazole, imidazole and oxazole containing amino acids useful for peptide synthesis)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1999:327923 CAPLUS
DOCUMENT NUMBER: 131:127509
TITLE: In vivo processing and antibiotic activity of microcin B17 analogs with varying ring content and altered bisheterocyclic sites
AUTHOR(S): Roy, Ranabir Sinha; Kelleher, Neil L.; Milne, Jill C.; Walsh, Christopher T.
CORPORATE SOURCE: Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Chemistry & Biology (1999), 6(5), 305-318
CODEN: CBOLE2; ISSN: 1074-5521
PUBLISHER: Current Biology Publications
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The Escherichia coli peptide antibiotic microcin B17 (MccB17) contains 4 oxazole and 4 thiazole rings and inhibits DNA gyrase. The role of individual and tandem pairs of heterocycles in bioactivity has not been determined previously. The 2 tandem 4,2-bisheterocycles in MccB17 were varied by expression of MccB17 or mutants containing altered sequences at Gly39-Ser40-Cys41 or Gly54-Cys55-Ser56. A mixture of 5-9-ring MccB17 isoforms were separated and quantitated for antibiotic potency. Mutagenesis of the thiazole-oxazole pair significantly affected antibiotic activity compared with the upstream oxazole-thiazole, which might stabilize partially cyclized intermediates against proteolysis. Enzymic heterocyclization in native MccB17 occurs distributively. Antibiotic activity correlates with the number of rings and is differentially sensitive to both the location and the identity of the 4,2-tandem heterocycle pairs in MccB17. Such tandem heterocycles might be useful pharmacophores in combinatorial libraries.
IT 84286-90-8DP, Microcin B17, analogs 234125-07-6P 234125-08-7P 234125-09-8P 234125-10-1P 234125-11-2P 234125-12-3P 234125-13-4P 234125-14-5P 234125-15-6P 234125-16-7P 234125-17-8P 234125-18-9P
RL: BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation)
(in vivo processing and antibiotic activity of microcin B17 analogs with varying ring content and altered bisheterocyclic sites)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 234125-07-6 CAPLUS

L31 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonyl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 234125-08-7 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2'-(aminomethyl)[2,4'-bithiazole]-4-carbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 234125-09-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2'-(aminomethyl)[2,4'-bioxazole]-4-carbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 234125-10-1 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonyl-L-asparaginyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 234125-11-2 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2'-(aminomethyl)[2,4'-bithiazole]-4-carbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 234125-12-3 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2'-(aminomethyl)[2,4'-bioxazole]-4-carbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 234125-13-4 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 234125-14-5 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 234125-15-6 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-(aminomethyl)-4-thiazolecarbonylglycylglycylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 234125-16-7 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 234125-17-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-

isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonyl-L-asparaginylglycylglycylglycylglycylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 234125-18-9 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginylglycylglycylglycylglycylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

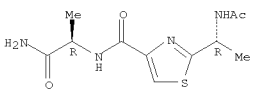
ACCESSION NUMBER: 1999:219066 CAPLUS
DOCUMENT NUMBER: 130:312089
TITLE: Ab initio calculations on peptide-derived oxazoles and thiazoles: improved molecular mechanics parameters for the AMBER force field
AUTHOR(S): Boden, Christopher D. J.; Pattenden, Gerald
CORPORATE SOURCE: Department of Chemistry, Nottingham University, Nottingham, NG7 2RD, UK
SOURCE: Journal of Computer-Aided Molecular Design (1999), 13(2), 153-166
CODEN: JCADEQ; ISSN: 0920-654X
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Ab initio calcns. at the RHF/6-31G* and MP2/6-31G*//RHF/6-31G* levels of theory are performed for 2-methyl-4-carboxamido-oxazoles and -thiazoles, including rotational profiles for the ring-carboxamide bond, which showed the expected conjugation and hydrogen bonding effects. On the basis of these data, newly optimized stretch, bend and torsional parameters for the AMBER* force field are derived, along with CHELPG-fitted partial atomic charges.

IT 223680-45-3 223680-49-7
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(ab initio calcns. on peptide-derived oxazoles and thiazoles)

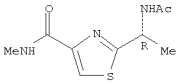
RN 223680-45-3 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-[(1R)-2-amino-1-methyl-2-oxoethyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 223680-49-7 CAPLUS
CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 31 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1999:212021 CAPLUS
DOCUMENT NUMBER: 131:40992
TITLE: Thiazole and oxazole peptides: biosynthesis and molecular machinery
AUTHOR(S): Roy, Ranabir Sinha; Gehring, Amy M.; Milne, Jill C.; Belshaw, Peter J.; Walsh, Christopher T.
CORPORATE SOURCE: Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Natural Product Reports (1999), 16(2), 249-263
CODEN: NPRRDF; ISSN: 0265-0568
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review, with 124 refs. Among the enzymic post-translational modifications of peptide-based natural products are heterocyclizations of serine, threonine, and cysteine side chains onto the preceding carbonyl groups to create five ring heterocycles in the oxazole and thiazole series. Initial products of cyclodehydration are the dihydroheteroarom. oxazolines and thiazolines which can undergo redox changes. A two-electron oxidation generates the heteroarom. oxazole and thiazole systems, while two electron redns. of the carbon-nitrogen double bonds would create the thiazolidine and oxazolidine rings. All three oxidation states are seen in natural products. The heterocyclizations not only alter peptide backbone connectivity and electronic distribution but also afford new recognition elements for interaction with such targets as DNA and RNA and with proteins that effect the specific biol. readouts of these natural products.
IT 84286-90-8, Microcin B17
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative)
(biosynthesis of thiazole and oxazole peptides)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 119 THERE ARE 119 CAPLUS RECORDS THAT CITE THIS RECORD (120 CITINGS)
REFERENCE COUNT: 124 THERE ARE 124 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 32 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1998:572745 CAPLUS
DOCUMENT NUMBER: 129:299581
ORIGINAL REFERENCE NO.: 129:61017a,61020a
TITLE: Regioselectivity and Chemoselectivity Analysis of Oxazole and Thiazole Ring Formation by the Peptide-Heterocyclizing Microcin B17 Synthetase Using High-Resolution MS/MS
AUTHOR(S): Kelleher, Neil L.; Belshaw, Peter J.; Walsh, Christopher T.
CORPORATE SOURCE: Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Journal of the American Chemical Society (1998), 120(37), 9716-9717
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The presence of rigid structural elements such as thiazole and oxazole heterocyclic rings in peptide-derived compds. confers a wide range of therapeutic properties including antibiotic, antiviral, and antitumor activity. Using high resolution tandem mass spectrometry (MS/MS), we determine here the effect of heterocycle formation on MS/MS of reaction intermediates and use this unique MS/MS signature to ascertain the regio- and chemoselectivity of microcin B17 synthetase.
IT 84286-90-8, Microcin B 17
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(regioselectivity and chemoselectivity anal. of oxazole and thiazole ring formation by peptide-heterocyclizing microcin B17 synthetase using high-resolution MS/MS)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 33 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1998:561978 CAPLUS
DOCUMENT NUMBER: 129:287745
ORIGINAL REFERENCE NO.: 129:58569a,58572a
TITLE: ATP/GTP hydrolysis is required for oxazole and thiazole biosynthesis in the peptide antibiotic microcin B17
AUTHOR(S): Milne, Jill C.; Eliot, Andrew C.; Kelleher, Neil L.; Walsh, Christopher T.
CORPORATE SOURCE: Department of Biological Chemistry, Molecular Pharmacology Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Biochemistry (1998), 37(38), 13250-13261
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In the maturation of the Escherichia coli antibiotic Microcin B17, the product of the mcbA gene is modified posttranslationally by the multimeric microcin synthetase complex (composed of McbB, C, and D) to cyclize four Cys and four Ser residues to four thiazoles and four oxazoles, resp. The purified synthetase shows an absolute requirement for ATP or GTP in peptide substrate heterocyclization, with GTP one-third as effective as ATP in initial rate studies. The ATPase/GTPase activity of the synthetase complex is conditional in that ADP or GDP formation requires the presence of substrate; noncyclizable versions of McbA bind to synthetase, but do not induce the NTPase activity. The stoichiometry of ATP hydrolysis and heterocycle formation is 5:1 for a substrate that contains two potential sites of modification. However, at high substrate concns. (>50Km) heteroocycle formation is inhibited, while ATPase activity occurs undiminished, consistent with uncoupling of NTP hydrolysis and heterocycle formation at high substrate concns. Sequence homol. reveals that the McbD subunit has motifs reminiscent of the Walker B box in ATP utilizing enzymes and of motifs found in small G protein GTPases. Mutagenesis of three aspartates to alanine in these motifs (D132, D147, and D199) reduced Microcin B17 production in vivo and heterocycle formation in vitro, suggesting that the 45 kDa McbD has a regulated ATPase/GTPase domain in its N-terminal region necessary for peptide heterocyclization.
IT 84286-90-8P, Microcin B17
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(ATP/GTP hydrolysis is required for oxazole and thiazole biosynthesis in peptide antibiotic microcin B17)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

L31 ANSWER 33 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 28 THERE ARE 28 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1998:482687 CAPLUS
DOCUMENT NUMBER: 129:231006
ORIGINAL REFERENCE NO.: 129:47015a
TITLE: Thrombin receptor (PAR-1) antagonists. Heterocycle-based peptidomimetics of the SFLLR agonist motif
AUTHOR(S): Hoekstra, William J.; Hulshizer, Becky L.; Mccomsey, David F.; Andrade-Gordon, Patricia; Kauffman, Jack A.; Addo, Michael F.; Oksenberg, Donna; Scarborough, Robert M.; Maryanoff, Bruce E.
CORPORATE SOURCE: The R. W. Johnson Pharmaceutical Research Institute, Spring House, PA, 19477, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1998), 8(13), 1649-1654
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
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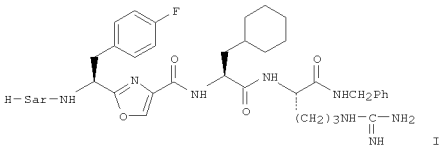


I

AB The thrombin receptor (PAR-1) is activated by α-thrombin to stimulate various cell types, including platelets, through the tethered-ligand sequence SFLLRN. A series of oxazole- or thiazole-based carboxamides, designed after SFLLR, were synthesized and evaluated in vitro. The compds. inhibited platelet aggregation induced by SFLLRN-NH2 or α-thrombin, and blocked the binding of [3H]-Ser-(p-F-Phe)-Har-Leu-Har-Lys-Tyr-NH2 (Har = homoarginine) to a CHRF membrane preparation of PAR-1. Oxazole-based peptide I bound to PAR-1 with an IC50 of 1.6 μM, and gave IC50 values of 25 μM and 6.6 μM against α-thrombin- and SFLLRN-NH2-induced platelet aggregation, resp.

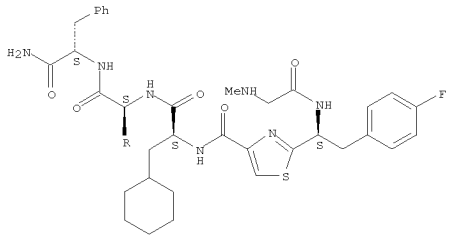
IT 212756-41-7P 212756-47-3P 212756-48-4P
212756-49-5P 212756-50-8P 212756-53-1P
212756-54-2P 212756-55-3P 212756-56-4P
212756-57-5P 212756-58-6P 212756-59-7P
212756-60-0P 212756-61-1P 212756-62-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of oxazole- and thiazole-based peptidomimetics as thrombin receptor antagonists)

RN 212756-41-7 CAPLUS

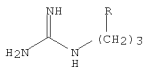
L31 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CN L-Phenylalaninamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

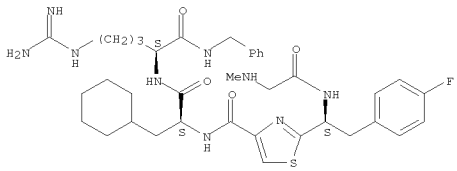


RN 212756-49-5 CAPLUS
CN L-Phenylalaninamide, L-valyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CN L-Argininamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

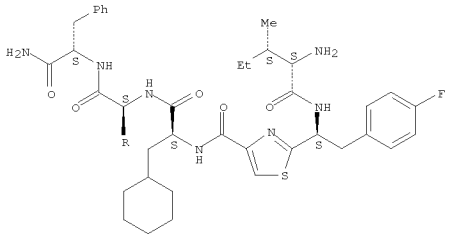
Absolute stereochemistry.



RN 212756-47-3 CAPLUS
CN L-Phenylalaninamide, L-isoleucyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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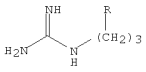
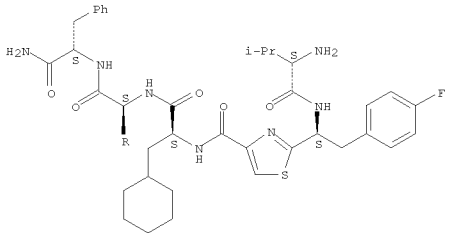


RN 212756-48-4 CAPLUS

L31 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A



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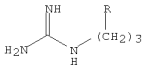
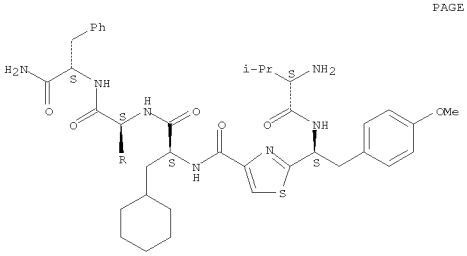


RN 212756-50-8 CAPLUS
CN L-Phenylalaninamide, L-valyl-2-[(1S)-1-amino-2-(4-methoxyphenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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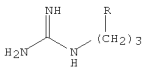
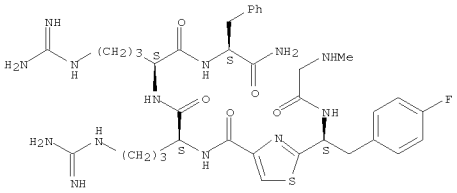


RN 212756-53-1 CAPLUS
CN L-Phenylalaninamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-L-arginyl-L-arginyl- (9CI) (CA INDEX NAME)

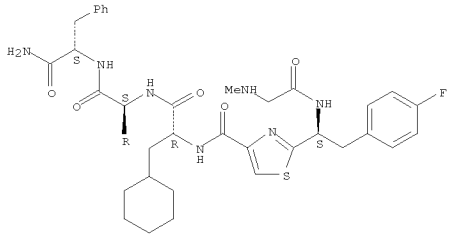
Absolute stereochemistry.



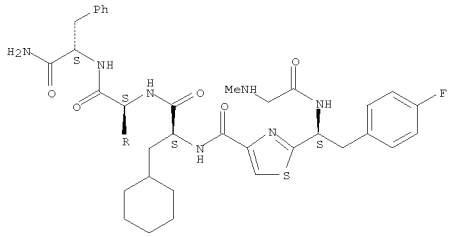
RN 212756-54-2 CAPLUS
CN L-Phenylalaninamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-D-alanyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

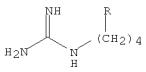
PAGE 1-A



PAGE 1-A

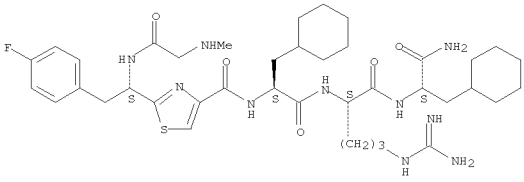


PAGE 2-A



RN 212756-57-5 CAPLUS
CN L-Alaninamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-L-arginyl-3-cyclohexyl- (9CI) (CA INDEX NAME)

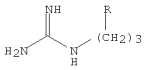
Absolute stereochemistry.



RN 212756-58-6 CAPLUS
CN Benzenebutanamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-L-arginyl-α-amino-, (αS)- (9CI) (CA INDEX NAME)

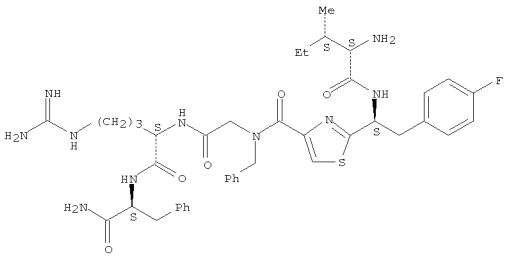
Absolute stereochemistry.

PAGE 2-A



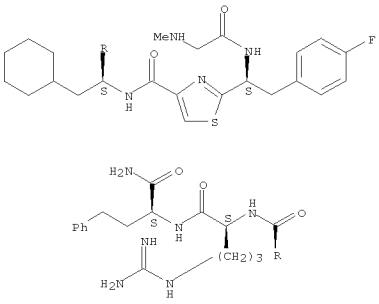
RN 212756-55-3 CAPLUS
CN L-Phenylalaninamide, L-isoleucyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-N-(phenylmethyl)glycyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



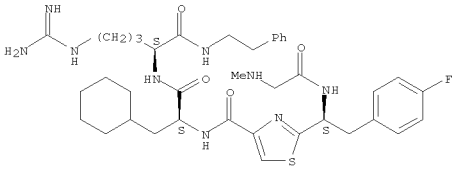
RN 212756-56-4 CAPLUS
CN L-Phenylalaninamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-N6-(aminoiminomethyl)-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



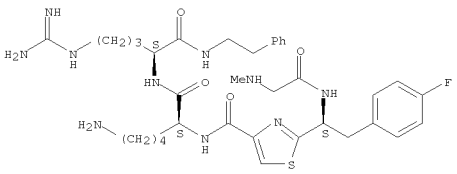
RN 212756-59-7 CAPLUS
CN L-Argininamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



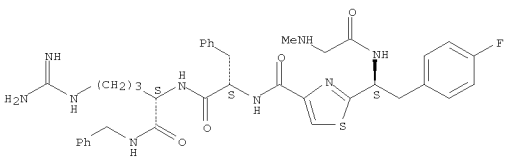
RN 212756-60-0 CAPLUS
CN L-Argininamide, N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-L-lysyl-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



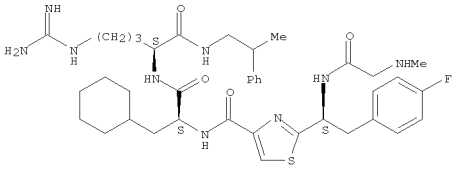
RN 212756-61-1 CAPLUS
CN L-Argininamide,
N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-L-phenylalanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 212756-62-2 CAPLUS
CN L-Argininamide,
N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarbonyl-3-cyclohexyl-L-alanyl-N-(2-phenylpropyl)- (9CI) (CA INDEX NAME)

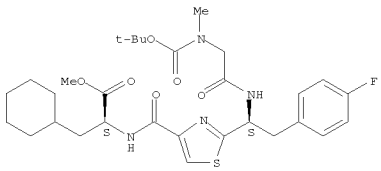
Absolute stereochemistry.



IT 212756-40-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of oxazole- and thiazole-based peptidomimetics as thrombin receptor antagonists)

RN 212756-40-6 CAPLUS
CN Cyclohexanepropanoic acid, α-[[[2-[(1S)-1-[[[[(1,1-dimethylethoxy)carbonyl]methylamino]acetyl]amino]-2-(4-fluorophenyl)ethyl]-4-thiazolyl]carbonyl]amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

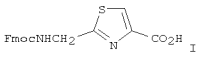


OS.CITING REF COUNT: 36 THERE ARE 36 CAPLUS RECORDS THAT CITE THIS RECORD (36 CITINGS)
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 35 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1998:147731 CAPLUS
DOCUMENT NUMBER: 128:291929
ORIGINAL REFERENCE NO.: 128:57747a,57750a
TITLE: Mutational analysis of posttranslational heterocycle biosynthesis in the gyrase inhibitor microcin B17: distance dependence from propeptide and tolerance for substitution in a GSCG cyclizable sequence
AUTHOR(S): Roy, Ranabir Sinha; Belshaw, Peter J.; Walsh, Christopher T.
CORPORATE SOURCE: Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Biochemistry (1998), 37(12), 4125-4136
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Microcin B17 (MccB17) is a peptidyl antibiotic that is secreted in stationary phase by several strains of Escherichia coli. The antibiotic efficacy of this polypeptide depends on the posttranslational modification of 8 cysteine and serine residues to thiazoles and oxazoles, resp., within the 69-amino acid McbA structural gene product. Mono- and bisheterocycle formation is mediated by MccB17 synthetase, an enzyme complex composed of 3 proteins: McbB, -C, and -D. After substrate processing, an N-terminal 26-amino acid propeptide sequence is cleaved to afford the mature antibiotic. A method for the overexpression and rapid purification of microcin synthetase was developed using a calmodulin-binding peptide tag. The determinants of substrate recognition and synthetase-mediated heterocycle formation were investigated by a systematic evaluation of 15 McbA1-46 analogs representing minimal substrates containing the first bisheterocyclization site (Gly39-Ser40-Cys41-Gly42) and variants thereof. Each substrate analog was overexpressed and affinity-purified as fusions to maltose-binding protein, incubated with purified synthetase, and evaluated for processing by Western blots, UV spectroscopy, and mass spectrometry. Insights gained into the process of enzymic heterocycle formation from cysteine and serine residues are discussed, including the distance dependence of the first cyclized residue from the propeptide and the local sequence context at the cyclizable sites. A model for McbA substrate recognition and processing by MccB17 synthetase is proposed.
IT 84286-90-8, Microcin B 17
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(mutational anal. of distance dependence from propeptide and tolerance for substitution in GSCG cyclizable sequence in posttranslational heterocycle biosynthesis of gyrase inhibitor microcin B17)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 36 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1996:639425 CAPLUS
DOCUMENT NUMBER: 125:329404
ORIGINAL REFERENCE NO.: 125:61719a,61722a
TITLE: Synthesis of all-thiazole microcin B17
AUTHOR(S): Videnov, G.; Ihlenfeldt, H. G.; Bayer, A.; Jung, G.
CORPORATE SOURCE: Institut fur Organische Chemie, Universitat Tubingen, Tuebingen, D-72076, Germany
SOURCE: Peptides 1994, Proceedings of the European Peptide Symposium, 23rd, Braga, Port., Sept. 4-10, 1994 (1995)
, Meeting Date 1994, 351-352. Editor(s): Maia, Hernani L. S. ESCOM: Leiden, Neth.
CODEN: 63MBAO
DOCUMENT TYPE: Conference
LANGUAGE: English
GI



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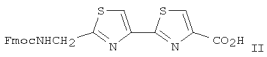


II

AB A report from a symposium on the solid-phase preparation of a microcin B17
analog in which all the oxazole rings are replaced with thiazole rings using thiazole and thioazolylthiazole building blocks I and II (Fmoc = 9-fluorenylmethoxycarbonyl).
IT 84286-90-8DP, Microcin B17, all-thiazole analog 183270-54-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase preparation of all-thiazole microcin B17)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-

(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 183270-54-4 CAPLUS
CN L-Isoleucine, N-[N-[N-[N-[[2-[[[[[[2-[[[N-[N2-[N-[N-[[2'-[[[N2-[N-[[2-[[[[[[2-[[[N-[N-[N2-[N-[N-[[2'-[[[N-[N-[N-[N-[N-[N-[N-[N-[N-[N-[N-L-

valylglycyl)-L-isoleucyl]glycyl]glycyl]glycyl]glycyl]glycyl]glycyl]glycyl]glycyl]

glycyl]glycyl]amino]methyl][2,4'-bithiazol]-4-yl]carbonyl]glycyl]glycyl]-L-glutaminyl]glycyl]glycyl]amino]methyl]-4-thiazolyl]carbonyl]amino]acetyl]amino]methyl]-4-thiazolyl]carbonyl]-L-seryl]-L-asparaginyl]amino]methyl][2,4'-bithiazol]-4-yl]carbonyl]glycyl]glycyl]-L-asparaginyl]glycyl]amino]methyl]-4-

thiazolyl]carbonyl]amino]acetyl]amino]methyl]-4-thiazolyl]carbonyl]glycyl]-

L-seryl]-L-histidyl]- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L31 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1996:616749 CAPLUS
DOCUMENT NUMBER: 126:8588
ORIGINAL REFERENCE NO.: 126:1911a,1914a
TITLE: Conformational Control by Thiazole and Oxazoline Rings in Cyclic Octapeptides of Marine Origin. Novel Macrocyclic Chair and Boat Conformations
AUTHOR(S): Abbenante, G.; Fairlie, D. P.; Gahan, L. R.; Hanson, G. R.; Pierens, G. K.; van den Brenk, A. L.
CORPORATE SOURCE: Centre for Drug Design and Development, University of Queensland, Brisbane, 4072, Australia
SOURCE: Journal of the American Chemical Society (1996), 118(43), 10384-10388
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

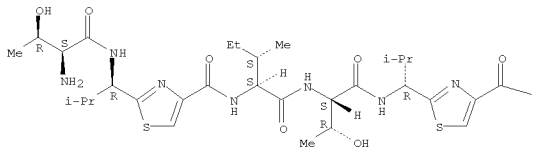
AB A comparison of a closely related set of cyclic octapeptides demonstrates how Nature has adapted two common amino acid building blocks (Thr, Cys) as
conformational ring constraints (oxazoline, thiazole) to regulate the three-dimensional structures and reactivities of marine macrocycles. A 2D NMR spectroscopic study shows that conversion of two Cys residues in the flexible cyclic octapeptide cyclo[Ile-Thr-D-Val-Cys-Ile-Thr-D-Val-Cys], to 5-membered thiazole rings (Thz) leads to the formation of a novel pseudochair conformation in I. The conformational flexibility of I is significantly restricted by three intramol. hydrogen bonds induced by the Thz components, resulting in
a single solution conformation with non-C2 sym. side chains. Addnl. modification, through conversion of the two Thr side chains to 5-membered oxazoline rings (Oxn), produces a highly constrained pseudoboat or saddle-shaped macrocycle II, having C2 sym. side chains. Acid hydrolysis of II, previously isolated from the ascidian Lissoclinum patella, selectively opens the two oxazoline rings with further conformational rearrangement to a novel cyclic depsipeptide III possessing a shallower pseudoboat conformation. The comparison reveals that oxazoline and thiazole rings impose severe conformational restrictions upon these cyclic octapeptides, creating unusual shapes and clefts with varying
capacities to capture organic or metal ion guests. Such dramatic changes in
macrocycle shape may be related to the differential antitumor and metal-binding properties of this class of mol.
IT 183613-10-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(macrocyclic chair and boat conformations induced by thiazole and oxazoline rings in cyclic octapeptides of marine origin)
RN 183613-10-7 CAPLUS
CN L-Isoleucine, L-threonyl-2-[(1R)-1-amino-2-methylpropyl]-4-

thiazolecarbonyl-L-isoleucyl-L-threonyl-2-[(1R)-1-amino-2-methylpropyl]-4-

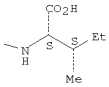
thiazolecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 35 THERE ARE 35 CAPLUS RECORDS THAT CITE THIS RECORD (35 CITINGS)
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 38 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1996:26661 CAPLUS
DOCUMENT NUMBER: 124:202085
ORIGINAL REFERENCE NO.: 124:37361a,37364a
TITLE: Synthesis of a Directly Connected Thiazole -Oxazole Ring System Present in Microcin B17
AUTHOR(S): Li, Gang; Warner, Philip M.; Jebaratnam, David J.
CORPORATE SOURCE: Department of Chemistry, Northeastern University, Boston, MA, 02115, USA
SOURCE: Journal of Organic Chemistry (1996), 61(2), 778-80
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The preparation of 2-[2-[(benzoylamino)methyl]-4-thiazolyl]-4-oxazolecarboxylic acid was described. This compound represents a ring system present in the 43 residue antibiotic microcin B17.
IT 84286-90-8DP, Microcin B17, ring system
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of microcin B17 ring system [(aminomethyl)thiazolyl]oxazolecarboxylate)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-

(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

L31 ANSWER 39 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
OS.CITING REF COUNT: 42 THERE ARE 42 CAPLUS RECORDS THAT CITE THIS RECORD (42 CITINGS)

L31 ANSWER 39 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1995:1007761 CAPLUS
DOCUMENT NUMBER: 124:255551
ORIGINAL REFERENCE NO.: 124:47236h,47237a
TITLE: Post-translational heterocyclic backbone modifications in the 43-peptide antibiotic microcin B17. Structure elucidation and NMR study of a 13C,15N-labeled gyrase inhibitor
AUTHOR(S): Bayer, Anja; Freund, Stefan; Jung, Guenther
CORPORATE SOURCE: Inst. Org. Chemie, Eberhard-Karls-Univ., Tuebingen, Germany
SOURCE: European Journal of Biochemistry (1995), 234(2), 414-26
CODEN: EJBCAI; ISSN: 0014-2956
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Microcin B17, the 1st known peptidic gyrase inhibitor, is produced by ribosomal synthesis and post-translational modification of the 69-residue precursor protein by an Escherichia coli strain. To elucidate the chemical structure of the mature 43-residue peptide antibiotic, fermentation and purification protocols were established and optimized which allow the isolation and purification of substantial amts. of highly pure B17 (non-labeled, 15N-labeled, and 13C/15N-labeled) peptide. By UV-absorption spectroscopy, HPLC-electrospray mass spectrometry, and GC-mass spectrometry, amino acid anal., protein sequencing, and, in particular, multidimensional NMR, it was proved that the enzymic modification of the precursor backbone at Gly-Cys and Gly-Ser segments leads to the formation of 2-aminomethylthiazole-4-carboxylic acid and 2-aminomethyloxazole-4-carboxylic acid, resp. In addition, 2 bicyclic modifications 2-(2-aminomethyloxazolyl)thiazole-4-carboxylic acid and 2-(2-aminomethylthiazolyl)oxazole-4-carboxylic acid, were found that consist of directly linked thiazole and oxazole rings derived from 1 Gly-Ser-Cys and 1 Gly-Cys-Ser segment. Analogous to the thiazole and oxazole rings found in antitumor peptides of microbial and marine origin, these heteroarom. ring systems of B17 presumably play an important role in its gyrase-inhibiting activity, e.g. interacting with the DNA to trap the covalent protein-DNA intermediate of the breakage-reunion reaction of the gyrase.
IT 84286-90-8, Microcin B17
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative)
(post-translational heterocyclic backbone modifications in microcin B17; structure elucidation and NMR study)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-

(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L31 ANSWER 40 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1994:529748 CAPLUS
DOCUMENT NUMBER: 121:129748
ORIGINAL REFERENCE NO.: 121:23345a,23348a
TITLE: Posttranslational modifications in microcin B17 define an additional class of DNA gyrase inhibitor
AUTHOR(S): Yorgey, Peter; Lee, Jonathan; Koerdel, Johann; Vivas, Eugenio; Warner, Philip; Jebaratnam, David; Kolter, Roberto
CORPORATE SOURCE: Dep. Microbiol., Harvard Med. Sch., Boston, MA, 02115, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1994), 91(10), 4519-23
CODEN: PNASA6; ISSN: 0027-8424
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Drugs that inhibit the activity of DNA gyrase fall almost exclusively into two structural classes, the quinolones and the coumarins. A third class of DNA gyrase inhibitor is defined by the ribosomally synthesized peptide antibiotic microcin B17 (MccB17). MccB17 contains 43 amino acid residues, but 14 of these are posttranslationally modified. Here the authors describe the characterization of the structure of these modifications. The authors propose that four cysteine and four serine side chains undergo condensation with the carbonyl group of the preceding residue, followed by α/β dehydrogenation to yield four thiazole and four oxazole rings, resp. The three proteins implicated in catalyzing these modifications (McbBCD) would constitute the only thiazole /oxazole biosynthetic enzymes identified. These results open up possibilities for the design of DNA gyrase inhibitors and add to the repertoire of posttranslational modifications with potential for protein engineering. Escherichia coli sbmA mutants, which lack the inner membrane protein (SbmA) involved in MccB17 uptake, were found to be resistant to bleomycin. Bleomycin is structurally unrelated to MccB17 except for the fact that it contains two thiazole rings. This suggests that thiazole rings are part of the MccB17 structure recognized by SbmA. This observation and the finding that SbmA homologs are widely conserved and can play developmental roles [Glazebrook, J., Ichige, A. & Walker, G. C. (1993) Genes Dev. 7,. 1485-1497] suggest that thiazole- and oxazole-containing compds. may serve as signaling mols. for a wide variety of bacteria in diverse environments, including pathogen interactions with plant and animal hosts.
IT 84286-90-8
RL: BIOL (Biological study)
(post-translational modification of serine and cysteine of, oxazole and thiazole moieties function in relation to)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-

L31 ANSWER 40 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
OS.CITING REF COUNT: 62 THERE ARE 62 CAPLUS RECORDS THAT CITE THIS RECORD (62 CITINGS)

L31 ANSWER 41 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1993:619696 CAPLUS
DOCUMENT NUMBER: 119:219696
ORIGINAL REFERENCE NO.: 119:39012h,39013a
TITLE: Post-translational backbone modification via heteroaromatic five-membered-ring formation during the biosynthesis of the glycine-rich antibiotic microcin B17
AUTHOR(S): Bayer, Anja; Freund, Stefan; Nicholson, Graeme; Jung, Guenther
CORPORATE SOURCE: Inst. Org. Chem., Univ. Tuebingen, Tuebingen, D-72076, Germany
SOURCE: Angewandte Chemie (1993), 105(9), 1410-13 (See also Angew. Chem., Int. Ed. Engl., 1993, 32(9), 1336-9)
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal; General Review
LANGUAGE: German
AB A review, with 14 refs., on the posttranslational modification of a peptide antibiotic, microcin B17, in which serine and cysteine residues undergo cyclization into 5-membered heterocyclic oxazole and thiazole rings.
IT 84286-90-8, Microcin B17
RL: PROC (Process)
(posttranslational modification of)
RN 84286-90-8 CAPLUS
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-

(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxazolecarbonylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (CA INDEX NAME)

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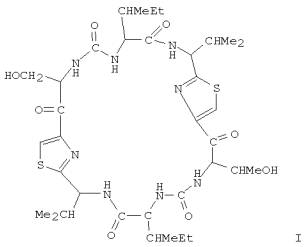
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

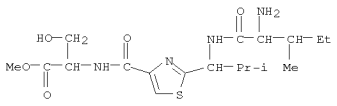
L31 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1993:473064 CAPLUS
DOCUMENT NUMBER: 119:73064
ORIGINAL REFERENCE NO.: 119:13193a,13196a
TITLE: Synthesis of the isomer of cyclopeptide ascidiacyclamide
AUTHOR(S): Jian, Zhigang; Jian, Dunlong; Long, Kanghou
CORPORATE SOURCE: Dep. Chem., Zhongshan Univ., Canton, 510275, Peop. Rep. China
SOURCE: Zhongshan Daxue Xuebao, Ziran Kexueban (1992), 31(2), 57-61
CODEN: CHTHAJ; ISSN: 0529-6579
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



I

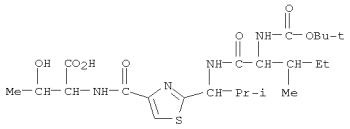
AB The title compound (I) has been synthesized. The thiazole amino acid was prepared by Hantzsch method. The peptide bonds were constructed by DCC-HOBT (DCC = dicyclohexylcarbodiimide, HOBT = 1-hydroxybenzatriazole hydrate) coupling method and the peptide ring was formed by azide method.
IT 148968-60-9P 148968-61-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling reaction of)
RN 148968-60-9 CAPLUS
CN L-Serine, L-isoleucyl-2-(1-amino-2-methylpropyl)-4-thiazolecarbonyl-, methyl ester, dihydrochloride (9CI) (CA INDEX NAME)

L31 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



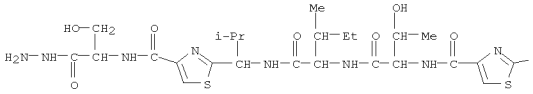
●2 HCl

RN 148968-61-0 CAPLUS
CN L-Threonine, N-[[2-[1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxopentyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]- (9CI) (CA INDEX NAME)



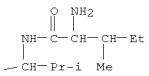
IT 135608-13-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 135608-13-8 CAPLUS
CN L-Isoleucinamide, N-[[2-[1-[(2-amino-3-methyl-1-oxopentyl)amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-L-threonyl-N-[1-[4-[[2-hydrazino-1-(hydroxymethyl)-2-oxoethyl]amino]carbonyl]-2-thiazolyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



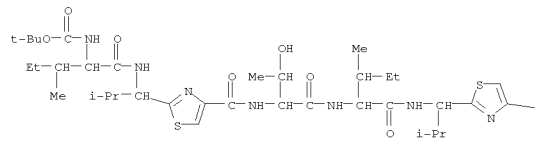
L31 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

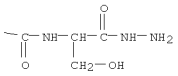


IT 135608-12-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 135608-12-7 CAPLUS
CN L-Isoleucinamide, N-[[2-[1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxopentyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-L-threonyl-N-[1-[4-[[[2-hydrazino-1-(hydroxymethyl)-2-oxoethyl]amino]carbonyl]-2-thiazolyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

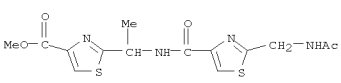


PAGE 1-B



IT 135608-11-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with hydrazine)
RN 135608-11-6 CAPLUS
CN L-Isoleucinamide, N-[[2-[1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxopentyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-L-threonyl-N-[1-[4-[[[1-(hydroxymethyl)-2-methoxy-2-oxoethyl]amino]carbonyl]-2-thiazolyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

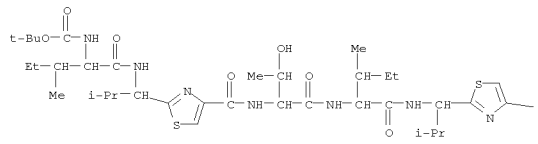
L31 ANSWER 43 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1992:546817 CAPLUS
DOCUMENT NUMBER: 117:146817
ORIGINAL REFERENCE NO.: 117:25365a,25368a
TITLE: The structures of A10255 B, -G and -J: new thiopeptide antibiotics produced by Streptomyces gardneri
AUTHOR(S): Debono, Manuel; Molloy, R. Michael; Occolowitz, John L.; Paschal, Jonathan W.; Hunt, Ann H.; Michel, Karl H.; Martin, James W.
CORPORATE SOURCE: Lilly Corp. Cent., Indianapolis, IN, 46285, USA
SOURCE: Journal of Organic Chemistry (1992), 57(19), 5200-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structures of the major members of a new family of important thiopeptide antibiotics, A10255B (I), A10255G (II), and A10255J (III), produced by S. gardneri (NRRL 15537) are described. Selective chemical degradation in combination with NMR, FABMS, and CID methods on the degradation products was required to solve these structures. Methanolysis of I resulted in the isolation of 4-carbomethoxy-2-propionyloxazole and di-Me sulfomycinamate as well as N-((acetamidomethyl)thiazolyl)-1-(carbomethoxythiazolyl)ethanamide after acetylation. Vigorous treatment with acid produced berninamycinic acid. Trifluoroacetolysis led to cleavage at the 6 dehydroalanine residues to give a complex and highly modified pentapeptide which was sequenced by CIDMS and NMR techniques. The pentapeptide was composed of sulfomycinamic acid, threonine, 1-(4-carboxyoxazolyl)-1-aminopentene unit (dehydronorvaline masked by oxazole at its carboxyl group), 2-(aminomethyl)thiazole -4-carboxylic acid, and 2-(1-aminoethyl)-4-carboxamidothiazole. FABMS and base hydrolysis showed that I had a dehydroalanine tetrapeptide side chain. Antibiotics II and III each had a masked dehydrobutyrin in place of the dehydronorvaline present in I, and III had a single amidated dehydroalanine as a side chain.
IT 143346-89-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 143346-89-8 CAPLUS
CN 4-Thiazolecarboxylic acid, 2-[1-[[[2-[(acetylamino)methyl]-4-thiazolyl]carbonyl]amino]ethyl]-, methyl ester (CA INDEX NAME)



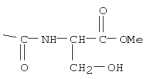
OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

L31 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B

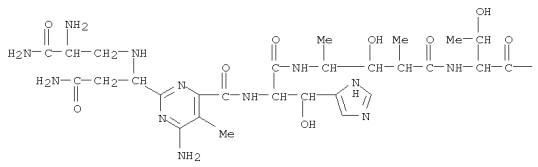


L31 ANSWER 44 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1992:512030 CAPLUS
DOCUMENT NUMBER: 117:112030
ORIGINAL REFERENCE NO.: 117:19579a,19582a
TITLE: On the role of individual bleomycin thiazoles in oxygen activation and DNA cleavage
AUTHOR(S): Hamamichi, Norimitsu; Natrajan, Anand; Hecht, Sidney M.
CORPORATE SOURCE: Dep. Chem. Biol., Univ. Virginia, Charlottesville, VA, 22901, USA
SOURCE: Journal of the American Chemical Society (1992), 114(16), 6278-91
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:112030
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Two structurally novel bleomycin (BLM) analogs I and II were prepared by total synthesis to permit the evaluation of the role of individual thiazole moieties in the processes of bleomycin-mediated oxygen activation and DNA degradation Each of the compds. was structurally related to deglycobleomycin demethyl A2 but contained an S-methyl-L-cysteine moiety in lieu of one of the two thiazoles normally present in bleomycin. In common with bleomycin and deglycobleomycin, both monothiazole BLMs were found to be excellent catalysts for the oxygenation of low mol. weight substrates such as naphthalene and styrene and also mediated the demethylation of N,N-dimethylaniline. However, both of the monothiazole BLMs were much less effective than bleomycin or deglycobleomycin in promoting DNA degradation Anal. of the effects of the monothiazole BLMs on 5'- and 3'-32P end labeled DNA duplexes indicated that cleavage occurred without discernible sequence selectivity. These results demonstrate that the bithiazole moiety in BLM is not required for O2 activation or for the oxygenation and oxidation of low mol. substrates in what are presumably biomol. processes. However, the bithiazole clearly does contribute to the efficiency of bleomycin-mediated DNA degradation and to the sequence selectivity of DNA strand scission by bleomycin.
IT 142721-45-7 142721-45-7D, iron complex
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxygen activation and DNA cleavage by)
RN 142721-45-7 CAPLUS
CN Bleomycinamide, 41-O-de[2-O-[3-O-(aminocarbonyl)-α-D-mannopyranosyl]-α-L-gulopyranosyl]-8,10-deepithio-7,8,10,11-tetrahydro-8-(methylthio)-N1-[3-(methylthio)propyl]-10-oxo-, (7S)- (9CI) (CA INDEX NAME)

PAGE 1-A



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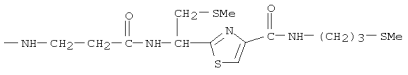
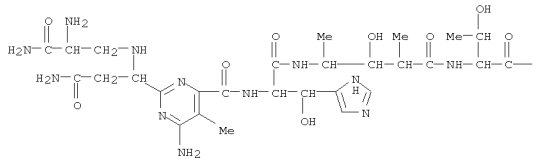


RN 142721-45-7 CAPLUS
CN Bleomycinamide, 41-O-de[2-O-[3-O-(aminocarbonyl)-α-D-mannopyranosyl]-α-L-gulopyranosyl]-8,10-deepithio-7,8,10,11-tetrahydro-8-(methylthio)-N1-[3-(methylthio)propyl]-10-oxo-, (7S)- (9CI) (CA INDEX NAME)

PAGE 1-A



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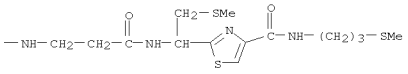

RN 142721-63-9 CAPLUS
CN β-Alaninamide, N-[(2,2,2-tribromoethoxy)carbonyl]-L-threonyl-N-[2-(methylthio)-1-[4-[[[3-(methylthio)propyl]amino]carbonyl]-2-thiazolyl]ethyl]-, (S)- (9CI) (CA INDEX NAME)

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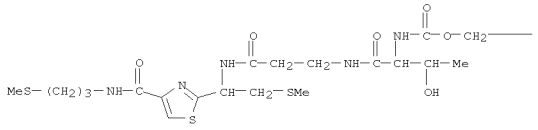

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RN 142721-65-1 CAPLUS
CN D-Arabinonamide, 2,4,5-trideoxy-4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-hydroxy-3-(1H-imidazol-4-yl)-1-oxopropyl]amino]-N-[2-hydroxy-1-[[[3-[[2-(methylthio)-1-[4-[[[3-(methylthio)propyl]amino]carbonyl]-2-thiazolyl]ethyl]amino]-3-oxopropyl]amino]carbonyl]propyl]-2-methyl-, [1[1S(S),2R],4(2S,3R)]-(9CI)
(CA INDEX NAME)

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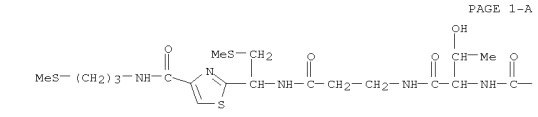

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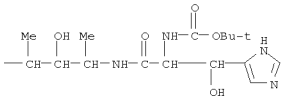

RN 142721-67-3 CAPLUS

IT 142721-66-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with pyrimidoblamic acid)
RN 142721-66-2 CAPLUS
CN D-Arabinonamide, 4-[[2-amino-3-hydroxy-3-(1H-imidazol-4-yl)-1-oxopropyl]amino]-2,4,5-trideoxy-N-[2-hydroxy-1-[[[3-[[2-(methylthio)-1-[4-[[[3-(methylthio)propyl]amino]carbonyl]-2-thiazolyl]ethyl]amino]-3-oxopropyl]amino]carbonyl]propyl]-2-methyl-, [1[1S(S),2R],4(2S,3R)]-(9CI)
(CA INDEX NAME)

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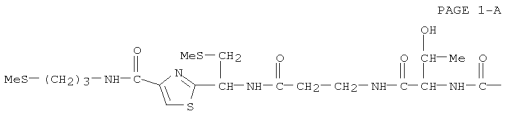
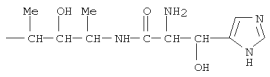
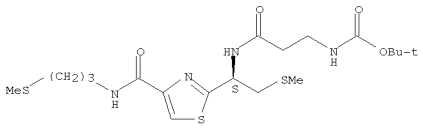


PAGE 1-B



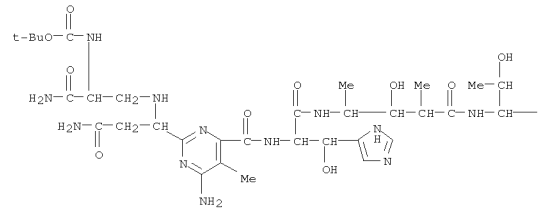
IT 142721-60-6P 142721-63-9P 142721-65-1P
142721-67-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)
RN 142721-60-6 CAPLUS
CN Carbamic acid, [3-[[2-(methylthio)-1-[4-[[[3-(methylthio)propyl]amino]carbonyl]-2-thiazolyl]ethyl]amino]-3-oxopropyl]-, 1,1-dimethylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

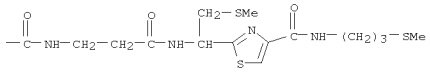


CN Bleomycinamide, 41-O-de[2-O-[3-O-(aminocarbonyl)-α-D-mannopyranosyl]-α-L-gulopyranosyl]-8,10-deepithio-N38-[(1,1-dimethylethoxy)carbonyl]-7,8,10,11-tetrahydro-8-(methylthio)-N1-[3-(methylthio)propyl]-10-oxo-, (7S)- (9CI) (CA INDEX NAME)

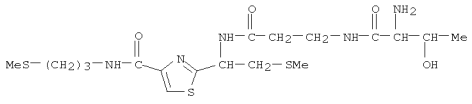
PAGE 1-A



PAGE 1-B

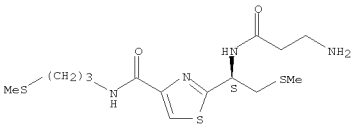


IT 142721-64-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and peptide coupling of, with dipeptide derivative)
RN 142721-64-0 CAPLUS
CN β-Alaninamide, L-threonyl-N-[2-(methylthio)-1-[4-[[[3-(methylthio)propyl]amino]carbonyl]-2-thiazolyl]ethyl]-, (S)- (9CI) (CA INDEX NAME)



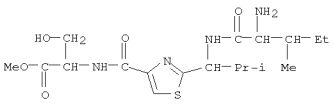
L31 ANSWER 44 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
IT 142721-61-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and peptide coupling of, with threonine derivative)
RN 142721-61-7 CAPLUS
CN 4-Thiazolecarboxamide, 2-[1-[(3-amino-1-oxopropyl)amino]-2-(methylthio)ethyl]-N-[3-(methylthio)propyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



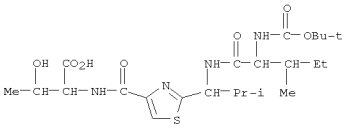
OS.CITING REF COUNT: 25 THERE ARE 25 CAPLUS RECORDS THAT CITE THIS RECORD (27 CITINGS)

L31 ANSWER 45 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

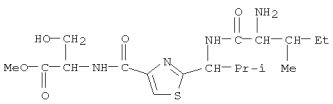


●2 HCl

RN 135607-99-7 CAPLUS
CN L-Threonine, N-[[2-[1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxopentyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-, [2S-[1(R*),2R*,3R*]]- (9CI) (CA INDEX NAME)



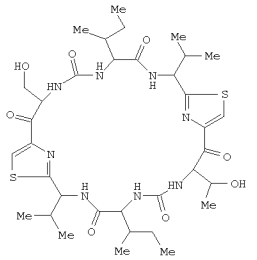
RN 135682-32-5 CAPLUS
CN L-Serine, L-isoleucyl-2-[(1R)-1-amino-2-methylpropyl]-4-thiazolecarbonyl-, methyl ester, dihydrochloride (9CI) (CA INDEX NAME)



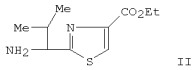
●2 HCl

RN 135682-34-7 CAPLUS
CN L-Threonine, N-[[2-[1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxopentyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-, [2S-[1(S*),2R*,3R*]]- (9CI) (CA INDEX NAME)

L31 ANSWER 45 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1991:515071 CAPLUS
DOCUMENT NUMBER: 115:115071
ORIGINAL REFERENCE NO.: 115:19753a,19756a
TITLE: Synthesis of cyclopeptide DL-(Val)Thz-L-Ser-L-Ile-L-ILE-L-Thr-DL-(Val)Thz
AUTHOR(S): Jian, Zhigang; Jian, Dunlong; Long, Kanghou
CORPORATE SOURCE: Dep. Chem., Zhongshan Univ., Canton, Peop. Rep. China
SOURCE: Zhongguo Haiyang Yaowu (1990), 9(3), 1-4
CODEN: ZHYAE8; ISSN: 1002-3461
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



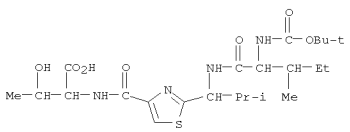
I



II

AB The title cyclopeptide (I) was prepared from L-serine, L-threonine, L-isoleucine, and thiazole II. Peptide ring was formed by azide method.
IT 135607-97-5P 135607-99-7P 135682-32-5P 135682-34-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling reaction of)
RN 135607-97-5 CAPLUS
CN L-Serine, L-isoleucyl-2-[(1S)-1-amino-2-methylpropyl]-4-thiazolecarbonyl-, methyl ester, dihydrochloride (9CI) (CA INDEX NAME)

L31 ANSWER 45 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



IT 135608-13-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 135608-13-8 CAPLUS
CN L-Isoleucinamide, N-[[2-[1-[(2-amino-3-methyl-1-oxopentyl)amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-L-threonyl-N-[1-[4-[[[2-hydrazino-1-(hydroxymethyl)-2-oxoethyl]amino]carbonyl]-2-thiazolyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

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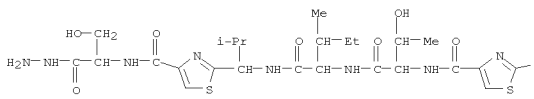

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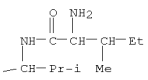
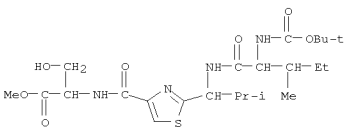


IT 135607-96-4P 135608-12-7P 135682-31-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 135607-96-4 CAPLUS
CN L-Serine, N-[[2-[1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxopentyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-, methyl ester, [2S-[1(R*),2R*,3R*]]- (9CI) (CA INDEX NAME)



RN 135608-12-7 CAPLUS
CN L-Isoleucinamide, N-[[2-[1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxopentyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-L-threonyl-N-[1-[4-[[[2-hydrazino-1-(hydroxymethyl)-2-oxoethyl]amino]carbonyl]-2-thiazolyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

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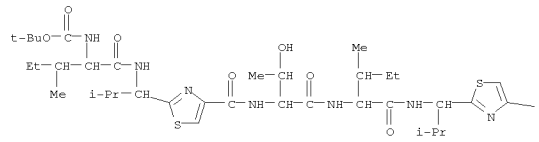
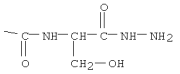
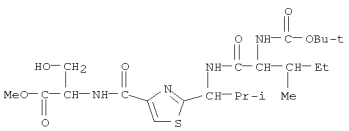


PAGE 1-B

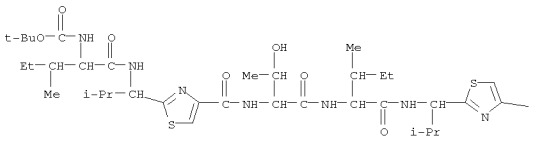


RN 135682-31-4 CAPLUS
CN L-Serine, N-[[2-[1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxopentyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-, methyl ester, [2S-[1(S*),2R*,3R*]]- (9CI) (CA INDEX NAME)

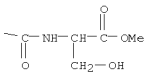


IT 135608-11-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with hydrazine)
RN 135608-11-6 CAPLUS
CN L-Isoleucinamide, N-[[2-[1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxopentyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-L-threonyl-N-[1-[4-[[[1-(hydroxymethyl)-2-methoxy-2-oxoethyl]amino]carbonyl]-2-thiazolyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

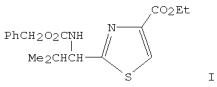
PAGE 1-A



PAGE 1-B



ACCESSION NUMBER: 1990:515828 CAPLUS
DOCUMENT NUMBER: 113:115828
ORIGINAL REFERENCE NO.: 113:19651a,19654a
TITLE: Synthesis of hexapeptide Ile-Thr-(Val)Thz-Ile-Thr-(Val)Thz
AUTHOR(S): Jian, Dunlong; Long, Kanghou
CORPORATE SOURCE: Chem. Dep., Zhongshan Univ., Canton, Peop. Rep. China
SOURCE: Yingyong Huaxue (1989), 6(5), 77-80
CODEN: YIHUED; ISSN: 1000-0518
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 113:115828
GI

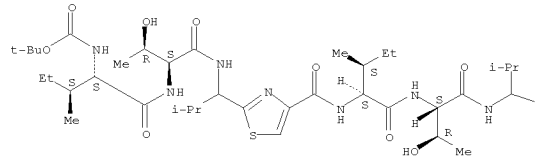


I

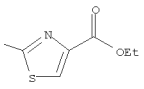
AB Hexapeptide Ile-Thr-(Val)Thz-Ile-Thr-(Val)Thz, the ring opening product of ascidiacyclamide, was synthesized. The (Val)Thiazole amino acid derivative I was prepared by Hantzsch method.
IT 128855-43-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 128855-43-6 CAPLUS
CN L-Threoninamide, N-[[2-[1-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-isoleucyl]-L-threonyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-L-isoleucyl-N-[1-[4-(ethoxycarbonyl)-2-thiazolyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L31 ANSWER 47 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1988:493623 CAPLUS
DOCUMENT NUMBER: 109:93623
ORIGINAL REFERENCE NO.: 109:15652h,15653a
TITLE: Preparation of thiazole- and tetrazole-containing peptides as renin inhibitors
INVENTOR(S): Raddatz, Peter; Gante, Joachim; Schmitges, Claus J.; Minck, Klaus Otto; Sombroek, Johannes; Hoelzemann, Guenter
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

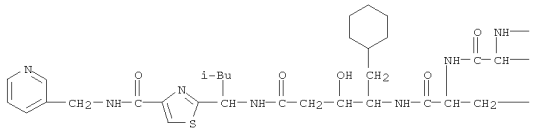
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3626130	A1	19880211	DE 1986-3626130	19860801
EP 262318	A2	19880406	EP 1987-110426	19870718
EP 262318	A3	19900411		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
AU 8776222	A	19880204	AU 1987-76222	19870727
AU 599401	B2	19900719		
CA 1298433	C	19920331	CA 1987-543473	19870730
JP 63041469	A	19880222	JP 1987-190577	19870731
ZA 8705692	A	19880427	ZA 1987-5692	19870731
US 4829053	A	19890509	US 1987-80265	19870731
HU 48642	A2	19890628	HU 1987-3536	19870731
HU 199506	B	19900228		

PRIORITY APPLN. INFO.: DE 1986-3626130 A 19860801

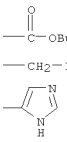
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 109:93623
AB X-Z-NR2CHR3CR4(CHR5)nCO-X1-NR6CHR7-D [I; X = H, R1SO2, R1O(CH2)mCO, R1(CH2)mO2C, etc.; Z = 0-4 amino acid residues; X1 = 0-2 amino acid residues; D = (substituted) tetrazolyl, thiazolyl; R1, R3, R7 = H, alkyl, aralkyl heteroaryl, (substituted) cycloalkyl, bicycloalkyl, etc; R2, R5, R6 = H, alkyl; R4 = (H, OH), (H, NH2), :O; n = 1,2; m = 0-5] were prepared as renin inhibitors (no data). 1-Bromo-3S-tert-butoxycarbonylamino-5-methylhexane-2-one was reacted with thiourea in MeOH to give 2-amino-4-(1S-tert-butoxycarbonylamino-3-methylbutyl) thiazole, which was deprotected and coupled with BOC-AHCP-OH, BOC-DNP-His-OH, and BOC-Phe-OH (BOC = tert-butoxycarbonylamino, ACHP = 4S-amino-3S-hydroxycyclohexylpentanoyl, DNP = 2,4-dinitrophenyl) followed by deprotection with 2-mercaptoethanol to give γ-amino-4-[1S-(3S-hydroxy-4S-(N-tert-butoxycarbonyl-L-phenylalanyl-L-histidylamino)-5-cyclohexylpentanoylamino)-3-methylbutyl]thiazole .
IT 115919-55-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as renin inhibitor)
RN 115919-55-6 CAPLUS
CN L-threo-Pentonamide, 5-cyclohexyl-2,4,5-trideoxy-4-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-N-[3-methyl-1-

L31 ANSWER 47 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
[4-[[(3-pyridinylmethyl)amino]carbonyl]-2-thiazolyl]butyl]-, (S)- (9CI) (CA INDEX NAME)

PAGE 1-A



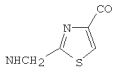
PAGE 1-B



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 48 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1988:132300 CAPLUS
DOCUMENT NUMBER: 108:132300
ORIGINAL REFERENCE NO.: 108:21723a,21726a
TITLE: The conformation of cyclo[L-Pro-L-Leu-L-Val-(gly)Thz-(gly)Thz], a dolastatin 3 analog, in the crystalline and solution states
AUTHOR(S): Stezowski, John J.; Poehlmann, Heinz W.; Haslinger, Ernst; Kalchhauser, Hermann; Schmidt, Ulrich; Pozolli, Bernd
CORPORATE SOURCE: Inst. Org. Chem., Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.
SOURCE: Tetrahedron (1987), 43(17), 3923-30
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:132300
GI

(gly)Thz =



AB The title peptide (I) was prepared in high yield via cyclization by the pentafluorophenyl active ester method. The crystal structure of I was determined I was also analyzed by 1H and 13C NMR in CDCl3 and DMSO-d6. The mol. adopts a preferred conformation in the crystal and in solution The conformation contains a cis (gly)Thz-Pro peptide bond and two intramol. hydrogen bonds, one from Leu-NH to a thiazole endocyclic nitrogen atom and the other from a (gly)Thz-NH to the Leu-CO. The results also provide conclusive evidence that the conformation proposed by J. L. Bernier, et al (1986) is incorrect. The crystal packing demonstrates that I is a very hydrophobic cyclopeptide with a tendency to self associate In the crystal I assocs. via systematic hydrogen bonding to form a network of interlocking hydrophobic tubes filled with toluene mols. The solvent mols. migrate out of the crystals on exposure to air resulting in fragmentation.
IT 104728-39-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with pentafluorophenol)
RN 104728-39-4 CAPLUS
CN L-Valinamide, 1-[(1,1-dimethylethoxy)carbonyl]-L-prolyl-L-leucyl-N-[[4-[[[(4-carboxy-2-thiazolyl)methyl]amino]carbonyl]-2-thiazolyl]methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 48 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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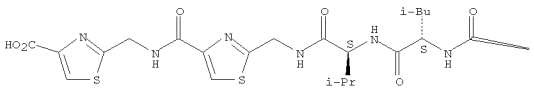

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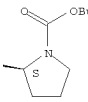

IT 113282-51-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 113282-51-2 CAPLUS
CN L-Valinamide, L-prolyl-L-leucyl-N-[[4-[[[[4-[(pentafluorophenoxy)carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 113282-50-1
CMF C32 H36 F5 N7 O6 S2

Absolute stereochemistry.

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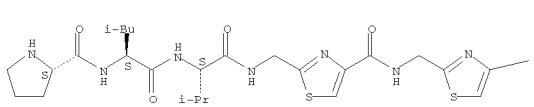

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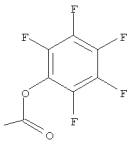


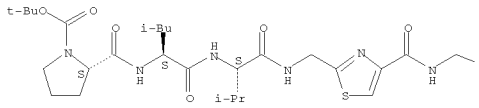
CM 2

CRN 76-05-1
CMF C2 H F3 O2

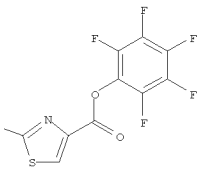
IT 113282-49-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)
RN 113282-49-8 CAPLUS
CN L-Valinamide, 1-[(1,1-dimethylethoxy)carbonyl]-L-prolyl-L-leucyl-N-[[4-[[[4-[(pentafluorophenoxy)carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L31 ANSWER 49 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1988:38343 CAPLUS
DOCUMENT NUMBER: 108:38343
ORIGINAL REFERENCE NO.: 108:6435a,6438a
TITLE: Amino acids and peptides. 60. Synthesis of biologically active cyclopeptides. 10. Synthesis of 16 structural isomers of dolastatin 3. II. Synthesis of the linear educts and the cyclopeptides
AUTHOR(S): Schmidt, Ulrich; Utz, Roland; Lieberknecht, Albrecht; Griesser, Helmut; Potzolli, Bernd; Bahr, Johanna; Wagner, Karin; Fischer, Peter
CORPORATE SOURCE: Isotopenforsch., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.
SOURCE: Synthesis (1987), (3), 236-41
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:38343
GI For diagram(s), see printed CA Issue.
AB Sixteen isomers (I and II) of the cancerostatic cyclopeptide dolastatin 3 were synthesized. The proposed structure of dolastatin 3 is shown by 1H NMR spectrometry to be incorrect.
IT 91711-92-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking-cyclization of)
RN 91711-92-1 CAPLUS
CN D-Valinamide, 1-[(1,1-dimethylethoxy)carbonyl]-D-prolyl-D-leucyl-N-[3-cyano-1-[4-[[[4-(ethoxycarbonyl)-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]propyl]-, (R)- (9CI) (CA INDEX NAME)

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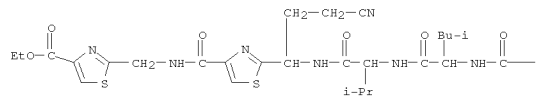
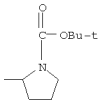


PAGE 1-B



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L31 ANSWER 50 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

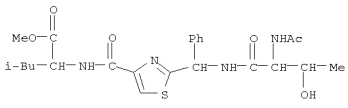
ACCESSION NUMBER: 1987:156837 CAPLUS
DOCUMENT NUMBER: 106:156837
ORIGINAL REFERENCE NO.: 106:25544h,25545a
TITLE: Total syntheses of patellamides, cytotoxic cyclic peptides from a marine tunicate
AUTHOR(S): Shibata, Makoto; Hamada, Yasumasa; Shioiri, Takayuki
CORPORATE SOURCE: Fac. Pharm. Sci., Nagoya City Univ., Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1985), 27th, 267-74
CODEN: TYKYDS
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The structures of patellamides A, B, and C have been proposed to be cyclic peptides I, II, and III, resp. I and II were synthesized by solution methods, but these synthetic peptides were not identical with natural patellamides B and C. An inspection of evidences used for the originally assigned structures and a synthetic study on the partial hydrolyzate of patellamide B indicated that the structures of patellamides B and C could be reassigned as cyclic peptides IV and V, resp., having the reverse order of amino acid residues. This deduction was confirmed by the syntheses of revised structures IV and V, which were completely identical with natural patellamides B and C, resp. The structures of patellamide A was analogously revised as cyclic peptide VI by its synthesis.

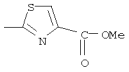
IT 106391-83-7
RL: PRP (Properties)
(mass spectrum of)

RN 106391-83-7 CAPLUS
CN L-Leucine, N-[[2-[[[2-(acetylamino)-3-hydroxy-1-oxobutyl]amino]phenylmethyl]-4-thiazolyl]carbonyl]-, methyl ester, [2S-[1(S*),2R*,3S*]]- (9CI) (CA INDEX NAME)

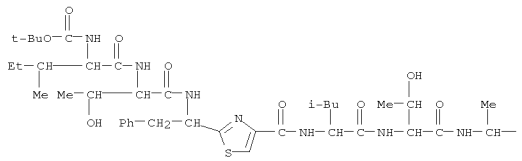


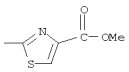
IT 101924-76-9P 101924-84-9P 102409-00-7P
103929-29-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking-cyclization of)

RN 101924-76-9 CAPLUS
CN L-Isoleucinamide, N-[[2-[1-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-allothreonyl]-L-leucyl]amino]-2-phenylethyl]-4-thiazolyl]carbonyl]-L-allothreonyl-N-[1-[4-(methoxycarbonyl)-2-thiazolyl]ethyl]-, [R-(R*,R*)]-



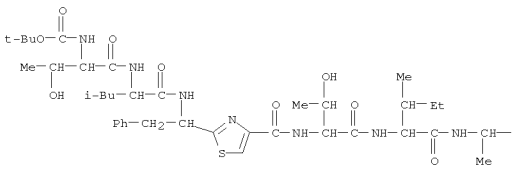
RN 102409-00-7 CAPLUS
CN L-Allothreoninamide, N-[[2-[1-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-isoleucyl]-L-allothreonyl]amino]-2-phenylethyl]-4-thiazolyl]carbonyl]-L-leucyl-N-[1-[4-(methoxycarbonyl)-2-thiazolyl]ethyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

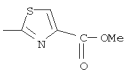




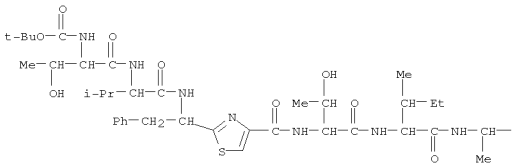
RN 103929-29-9 CAPLUS
CN L-Serinamide, N-[[2-[1-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-isoleucyl]-L-allothreonyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-L-isoleucyl-N-

(9CI) (CA INDEX NAME)

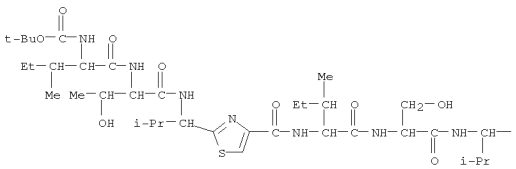


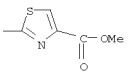


RN 101924-84-9 CAPLUS
CN L-Isoleucinamide, N-[[2-[1-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-allothreonyl]-L-valyl]amino]-2-phenylethyl]-4-thiazolyl]carbonyl]-L-allothreonyl-N-[1-[4-(methoxycarbonyl)-2-thiazolyl]ethyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)



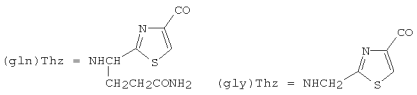
[1-[4-(methoxycarbonyl)-2-thiazolyl]-2-methylpropyl]-, [R-(R*,R*)]- (9CI)
(CA INDEX NAME)





L31 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1986:627283 CAPLUS
DOCUMENT NUMBER: 105:227283
ORIGINAL REFERENCE NO.: 105:36727a,36730a
TITLE: Structural biochemistry. 25. Antineoplastic agents. 110. Synthesis of the dolastatin 3 isomer cyclo[L-Pro-L-Leu-L-Val-(R,S)-(gln)Thz-(gly)Thz]
AUTHOR(S): Pettit, George R.; Holzapfel, Cedric W.
CORPORATE SOURCE: Cancer Res. Inst., Arizona State Univ., Tempe, AZ, 85287, USA
SOURCE: Journal of Organic Chemistry (1986), 51(24), 4580-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:227283
GI



AB The title cyclic peptide (I) was prepared by deblocking Boc-L-Leu-L-Val-(R,S)-(gln)Thz-(gly)Thz-L-Pro-OC6H2Cl3-2,4,5 (II, Boc = Me3CO2C) by CF3CO2H and cyclizing the resulting Boc-deblocked peptide in THF containing pyridine. II was prepared by solution methods. A comparison of synthetic I with natural dolastatin 3 showed that the natural peptide possesses a different absolute configuration arising from some D epimers of the amino acid residues. 1H and 13C NMR data indicated that dolastatin 3 may contain D-Leu and (R)-(glu)Thz.

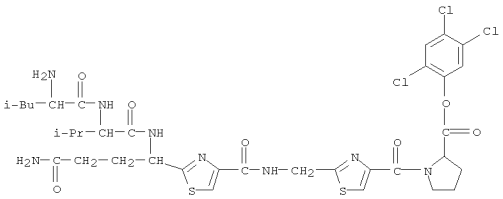
IT 104619-65-0P 104712-90-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 104619-65-0 CAPLUS
CN L-Valinamide, L-leucyl-N-[4-amino-4-oxo-1-[4-[[[[4-[[2-[(2,4,5-trichlorophenoxy)carbonyl]-1-pyrrolidinyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]butyl]-, [S-(R*,S*)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 104619-64-9
CMF C35 H43 Cl3 N8 O7 S2

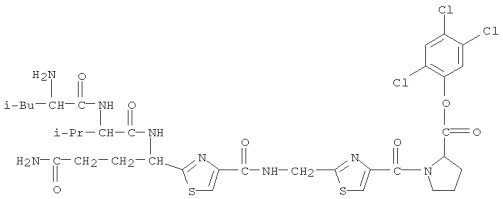
L31 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

L31 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 1

CRN 104712-89-2
CMF C35 H43 Cl3 N8 O7 S2

L31 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

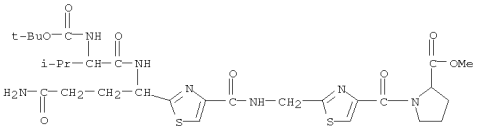
CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT 92506-94-0P 104619-59-2P 104619-61-6P
104619-62-7P 104619-63-8P 104712-82-5P
104712-84-7P 104712-85-8P 104712-86-9P
104712-87-0P 104712-88-1P 104757-49-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for dolastatin 3 stereoisomer)

RN 92506-94-0 CAPLUS
CN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-N-[4-amino-1-[4-[[[[4-[[2-(methoxycarbonyl)-1-pyrrolidinyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]-4-oxobutyl]-, [S-(R*,R*)]-(9CI) (CA INDEX NAME)

RN 104619-59-2 CAPLUS
CN L-Proline, 1-[[2-[[[[2-[4-amino-1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxobutyl]amino]-4-oxobutyl]-4-thiazolyl]carbonyl]amino]methyl]-4-thiazolyl]carbonyl]-, methyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)



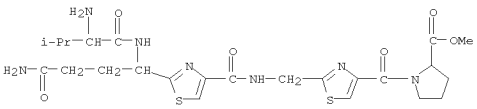
RN 104619-61-6 CAPLUS

L31 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CN L-Proline, 1-[[2-[[[[2-[4-amino-1-[(2-amino-3-methyl-1-oxobutyl)amino]-4-oxobutyl]-4-thiazolyl]carbonyl]amino]methyl]-4-thiazolyl]carbonyl]-, methyl ester, [R-(R*,S*)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

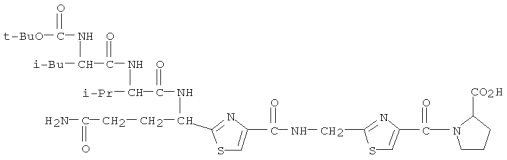
CRN 104619-60-5
CMF C24 H33 N7 O6 S2



CM 2

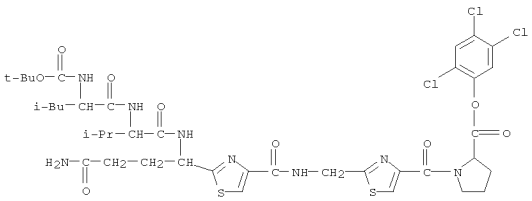
CRN 76-05-1
CMF C2 H F3 O2

RN 104619-62-7 CAPLUS
CN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-N-[4-amino-1-[4-[[[[4-[(2-carboxy-1-pyrrolidinyl)carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]-4-oxobutyl]-, [S-(R*,S*)]-(9CI) (CA INDEX NAME)

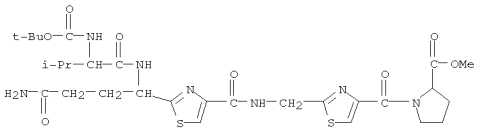


RN 104619-63-8 CAPLUS
CN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-N-[4-amino-4-oxo-1-[4-[[[[4-[[2-[(2,4,5-trichlorophenoxy)carbonyl]-1-pyrrolidinyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]butyl]-, [S-(R*,S*)]- (9CI)

(CA INDEX NAME)



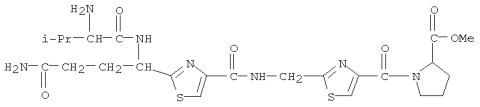
RN 104712-82-5 CAPLUS
CN L-Proline, 1-[[2-[[[[2-[4-amino-1-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methyl-1-oxobutyl]amino]-4-oxobutyl]-4-thiazolyl]carbonyl]amino]methyl]-4-thiazolyl]carbonyl]-, methyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)



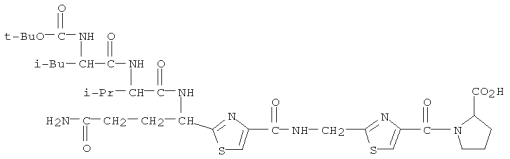
RN 104712-84-7 CAPLUS
CN L-Proline, 1-[[2-[[[[2-[4-amino-1-[(2-amino-3-methyl-1-oxobutyl)amino]-4-oxobutyl]-4-thiazolyl]carbonyl]amino]methyl]-4-thiazolyl]carbonyl]-, methyl ester, [S-(R*,R*)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

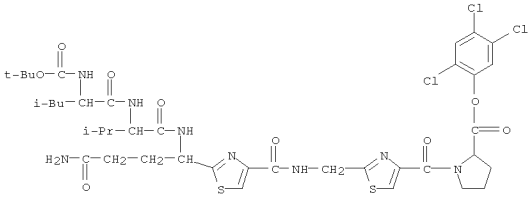
CRN 104712-83-6
CMF C24 H33 N7 O6 S2



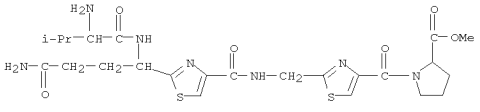
CM 2



RN 104712-88-1 CAPLUS
CN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-N-[4-amino-4-oxo-1-[4-[[[[4-[[2-[(2,4,5-trichlorophenoxy)carbonyl]-1-pyrrolidinyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]butyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)



RN 104757-49-5 CAPLUS
CN L-Proline, 1-[[2-[[[[2-[4-amino-1-[(2-amino-3-methyl-1-oxobutyl)amino]-4-oxobutyl]-4-thiazolyl]carbonyl]amino]methyl]-4-thiazolyl]carbonyl]-, methyl ester, monohydrobromide, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

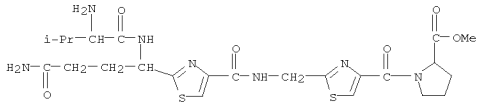


● HBr

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD

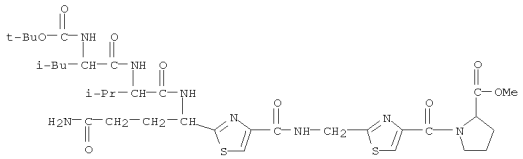
CRN 76-05-1
CMF C2 H F3 O2

RN 104712-85-8 CAPLUS
CN L-Proline, 1-[[2-[[[[2-[4-amino-1-[(2-amino-3-methyl-1-oxobutyl)amino]-4-oxobutyl]-4-thiazolyl]carbonyl]amino]methyl]-4-thiazolyl]carbonyl]-, methyl ester, monohydrobromide, [R-(R*,S*)]- (9CI) (CA INDEX NAME)



● HBr

RN 104712-86-9 CAPLUS
CN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-N-[4-amino-1-[4-[[[[4-[[2-(methoxycarbonyl)-1-pyrrolidinyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]-4-oxobutyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)



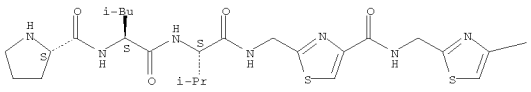
RN 104712-87-0 CAPLUS
CN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-N-[4-amino-1-[4-[[[[4-[[2-carboxy-1-pyrrolidinyl)carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]-4-oxobutyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

L31 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1986:573028 CAPLUS
DOCUMENT NUMBER: 105:173028
ORIGINAL REFERENCE NO.: 105:27904h,27905a
TITLE: Analog of dolastatin 3. Synthesis, proton NMR studies, and spatial conformation
AUTHOR(S): Bernier, Jean Luc; Houssin, Raymond; Henichart, Jean Pierre
CORPORATE SOURCE: INSERM, Lille, 59045, Fr.
SOURCE: Tetrahedron (1986), 42(10), 2695-702
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:173028
GI For diagram(s), see printed CA Issue.
AB Dolastatin 3 analog I was prepared by deblocking Boc-Pro-Leu-Val-(gly)Thz-(gly)Thz-ONSu (II; Boc = Me3CO2C, NSu = succinimido) by HBr/HOAc and cyclizing the resulting H-Pro-Leu-Val-(gly)Thz-(gly)Thz-ONSu.HBr in pyridine. Boc-Gly-NH2 underwent thionation via the Lawesson procedure to give Boc-Gly(S)-NH2, which was cyclized with CH3COCO2Et to give Boc-(gly)Thz-OEt (III). III was Boc-deblocked by HBr/HOAc to give H-(gly)Thz-OEt.HBr (IV), whereas III was saponified to give Boc-(gly)Thz-OH (V). V was coupled with IV by DCC/HOBt to give Boc-(gly)Thz-(gly)Thz-OEt, which was Boc-deblocked and then coupled with Boc-Pro-Leu-Val-OH by DCC/HOBt to give Boc-Pro-Leu-Val-(gly)Thz-(gly)Thz-OEt, which was converted into II. A spatial mol. conformation of I was proposed based on 1H NMR spectroscopy.
IT 104728-46-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 104728-46-3 CAPLUS
CN L-Valinamide, L-prolyl-L-leucyl-N-[[4-[[[4-[[(2,5-dioxo-1-pyrrolidinyl)oxy]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-, monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

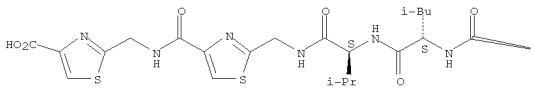


● HBr

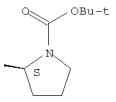
L31 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

Absolute stereochemistry.

PAGE 1-A



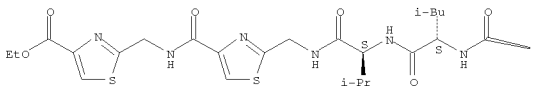
PAGE 1-B



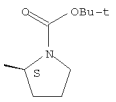
IT 104728-38-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and saponification of)
RN 104728-38-3 CAPLUS
CN L-Valinamide, 1-[(1,1-dimethylethoxy)carbonyl]-L-prolyl-L-leucyl-N-[[4-[[[4-(ethoxycarbonyl)-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



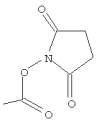
PAGE 1-B



IT 104728-40-7P

L31 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

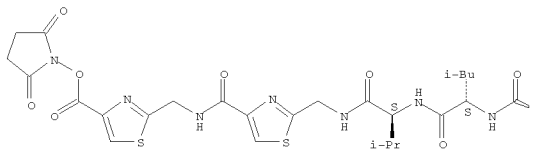
PAGE 1-B



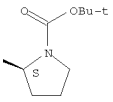
IT 104728-45-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)
RN 104728-45-2 CAPLUS
CN L-Valinamide, 1-[(1,1-dimethylethoxy)carbonyl]-L-prolyl-L-leucyl-N-[[4-[[[[4-[[(2,5-dioxo-1-pyrrolidinyl)oxy]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

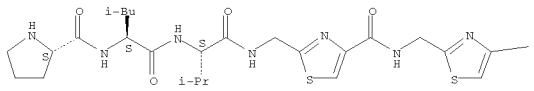


IT 104728-39-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and esterification with hydroxysuccinimide)
RN 104728-39-4 CAPLUS
CN L-Valinamide, 1-[(1,1-dimethylethoxy)carbonyl]-L-prolyl-L-leucyl-N-[[4-[[[(4-carboxy-2-thiazolyl)methyl]amino]carbonyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

L31 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 104728-40-7 CAPLUS
CN L-Valinamide, L-prolyl-L-leucyl-N-[[4-[[[(4-carboxy-2-thiazolyl)methyl]amino]carbonyl]-2-thiazolyl]methyl]-, monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● HBr

PAGE 1-B

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L31 ANSWER 53 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1984:552333 CAPLUS
DOCUMENT NUMBER: 101:152333
ORIGINAL REFERENCE NO.: 101:23083a,23086a
TITLE: Amino acids and peptides. Part 47. Synthesis of a compound whose structure was proposed as dolastatin 3
AUTHOR(S): Schmidt, Ulrich; Utz, Roland
CORPORATE SOURCE: Inst. Org. Chem., Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.
SOURCE: Angewandte Chemie (1984), 96(9), 723-4
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

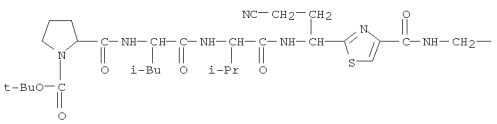
AB Cyclic peptide I (R = CONH2) (II), a proposed structure for dolastatin 3, was prepared by deblocking peptide III (Boc = Me3CO2C) by CF3CO2H, cyclizing the resulting Boc-deblocked peptide, and hydrolyzing the resulting I (R = CN). Thioamide IV was cyclized BrCH2COCO2Et to give thiazole V, which was cleaved by NH3 to give thiazole VI (R1 = CONH2, R2 = OH), which converted to VI [R1 = CN, R2 = Boc-(R)-Val-NH] (VII) in 5 steps. VII was Boc-deblocked and then coupled with Boc-(R)-Pro-(R)-Leu-OH to give VI [R1 = CN, R2 = Boc-(R)-Pro-(R)-Leu-(R)-Val-NH], which was converted to III in 3 steps. II was not identical with dolastatin 3.

IT 91741-74-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking-cyclization of)

RN 91741-74-1 CAPLUS

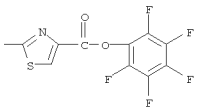
CN D-Valinamide, 1-[(1,1-dimethylethoxy)carbonyl]-D-prolyl-D-leucyl-N-[3-cyano-1-[4-[[[[4-[(pentafluorophenoxy)carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]propyl]-, (R)- (9CI) (CA INDEX NAME)

PAGE 1-A



L31 ANSWER 53 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

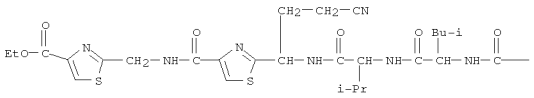


IT 91711-92-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and saponification-pentafluorophenyl esterification of)

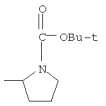
RN 91711-92-1 CAPLUS

CN D-Valinamide, 1-[(1,1-dimethylethoxy)carbonyl]-D-prolyl-D-leucyl-N-[3-cyano-1-[4-[[[[4-(ethoxycarbonyl)-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]propyl]-, (R)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     269.98    1694.79

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                     -45.05     -53.55

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